ACD/ChemSketch

Version 11.0 for Microsoft Windows

Reference Manual

Comprehensive Interface Description

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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 with the default Windows Display Properties.

This reference manual is provided in electronic form, readable with Adobe Acrobat 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* or left-click means point to an item, and press the left mouse button.
- *Right-click* means point to an item, and press the right mouse button.
- *Double-click* means point to an item, and quickly press 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 by either 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. As of Autumn 2007, we offer free ChemSketch 11.0, an ACD/Log*P* 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 ChemSketch) available for download.

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 page.

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/feedback/mailing.html

If you would like to participate in the ACD/Labs forums, please access:

http://forum.acdlabs.com

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.com

Technical and scientific support issues should be addressed by visiting:

http://support.acdlabs.com

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

All PC-based 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. The updates are small fixes, for example, bringing the actual version number of a program from 11.00 to 11.01. For more information on this, please refer to the document located in the ACD/Labs documentation folder, \\DOCS\UP_CLNT.PDF, or contact our technical support department.

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1. Introduction

1.1 About ACD/ChemSketch

ACD/ChemSketch is the powerful all-purpose chemical drawing and graphics package from ACD/Labs developed to help chemists quickly and easily draw molecular 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 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 (can be downloaded from **http://www.acdlabs.com/**). ACD/ChemBasic is available as part of the ACD/ChemSketch freeware download on our Web site. For examples on how ChemBasic can be used with ChemSketch, refer to Appendix C, "Goodies".

- **ACD/I-Lab**—the Internet-based service that allows you to get instant access to chemical databases and property predictions programs. An account on the Interactive Lab can be set up from **http://www.acdlabs.com/ilab**. As of Spring 2005, a 2-week demo period can be arranged for ACD/I-Lab. ACD/ChemSketch 8.0 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 structures (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!*** The new version of ACD/Dictionary contains more than 125,000 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 (ACD/Dictionary included in the commercial version only). For more information, refer to Section 3.13.6.

- **ACD/Name Freeware—**generates a name for structure 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 boiling points at any pressure from 0.001 torr to 7600 torr, in most cases to ±10 degrees or better, for a structure as drawn in the ChemSketch window. This additional application is described in the separate *ACD/Boiling Point User's Guide* (\\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* (\\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* (\\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 11.0

General Capabilities

- Generation of InChI key and auxiliary information on InChI

- Applying antialiasing

- Improved zoom

- Possibility to view all of the supported formats at once when opening documents

- New Document button is added to the existing command

- Some shortcuts are changed in accordance with MS Windows standard

Structure Mode

- ACD/Labs now supports a usage of special coordination bonds that represent a specific bonding between a ligand and metal center in coordination structures. Such bonds indicate a connection but do not affect the valence of the corresponding atoms.
Version 10.0 *vs.* version 11.0:
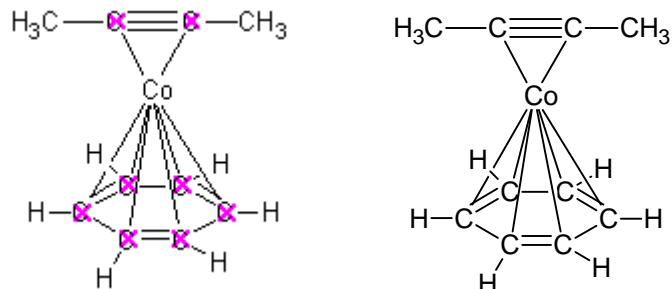
- Simplified usage of structure drawing styles

- Possibility to use both superscript and subscript characters in the same label.

Draw Mode

- Ability to insert and export images with .PNG extension

- Editing of the previously inserted text using the same tool

1.4 Freeware Version

From April 1999 onward, ACD/Labs has been making ChemSketch available as freeware, through the "Free Stuff" link at our Web site.

Now version 11.0 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 Freeware and also the Frequently Asked Questions (FAQs) can be found on our Web site at **http://www.acdlabs.com/products/chem_dsn_lab/chemsketch/tech.html**.

> **Note** Although ACD/ChemSketch freeware does not entitle you to technical support, we encourage you to visit the ChemSketch newsgroup where you can post your questions or share tips.
> **http://forum.acdlabs.com**

2. Interface Overview

2.1 Objectives

This chapter will familiarize you with the ChemSketch window and its basic elements.

Instructions for system requirements, and for installing and uninstalling the software are provided on a separate sheet of paper, shipped with the software itself.

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 each toolbar 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** SS Search will start the substructure search and as a result will automatically switch to the Database window displaying the search result.

2.2.1 Toolbar Customization

The toolbars of each ACD/Labs program can be customized by right-clicking the toolbar. The following options are available on the context menu that appears.

- Toolbar buttons—you can cancel the selection of a button to hide it.
- **Reset Toolbar**—selects all of the toolbar buttons on the list.

If some of the buttons do not fit, **More Buttons** " appears on the toolbar. Some of the toolbars display the shortcut menu containing the following additional commands:

- **Chevron Style**—adds **More Buttons** " at the end of the toolbar if the buttons do not fit on the toolbar.
- **Wrap Style**—splits the toolbar into two parts (one under another) if the buttons do not fit on the toolbar.
- **Gray Scale Style**—switches on/off the toolbar buttons' coloration.
- **Colored Highlight**—switches on/off the coloration of the selected buttons (when a button is pressed or the mouse pointer is placed on a button).

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 NONAME*XX*.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:

Buttons	Description
_	**Minimize** button—reduces the window. Note that this option is available only if the window is not already minimized.
🗗	**Restore** button—returns the window to its previous size. Note that this option is available only if the window is maximized.
🗖	**Maximize** button—makes the window fill the entire screen. Note that this option is available only if the desktop or window is not already maximized.
✕	**Close** button—closes all of the opened documents. If you have made any changes to the opened document and haven't saved your work yet, the program prompts you to do so.
🖼	**Control Menu** box—displays the shortcut menu with the listed above commands.

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** 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 and Reactive Reports and any other RSS channels specified by you.

> **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 this dialog box, on the RSS News bar, click Setup RSS .
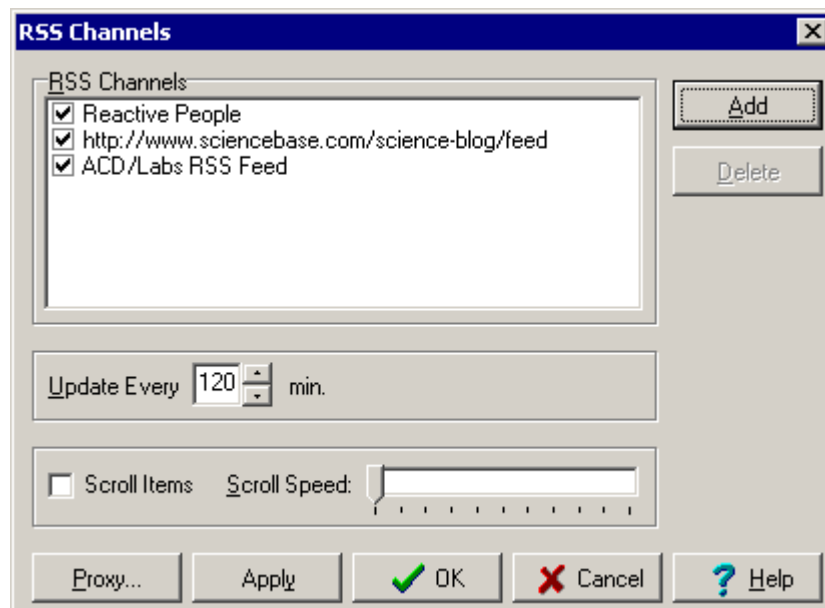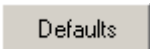
Option	Description
RSS Channels	Displays a list of RSS channels. Select the check boxes of the channels you want to be displayed.
	Note that ACD/Labs RSS Feed and Reactive People news cannot be switched off.
Add	Click this button to add the new URL to the **RSS Channels** list.
Delete	Click this button 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.
Update Every…min.	Specify the interval of information renewal (in the range from 1 to 120 minutes).
Scroll Items	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.
Scroll Speed	Move the slider left or right to set the speed of scrolling.
Proxy...	Displays the **HTTP Proxy Parameters** dialog box. For more information refer to Section 2.5.2.
Apply	Click this button to apply the specified settings without closing the dialog box.

2.5.2 HTTP Proxy Parameters Dialog Box

This dialog box allows you to specify parameters of the Proxy Server if the latter is required.
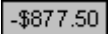
To display this dialog box, in the **RSS Channels** dialog box, click **Proxy** Proxy....
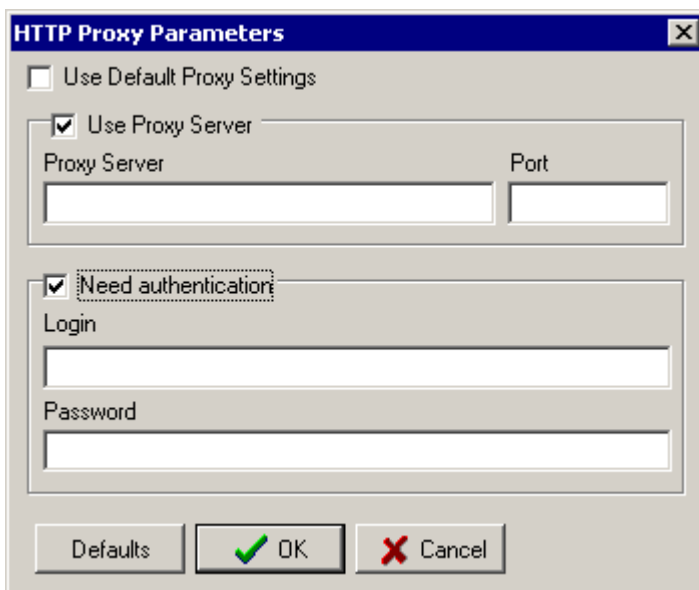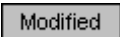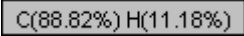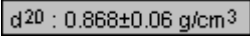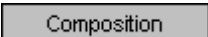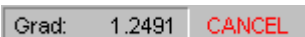
Option	Description
Use Default Proxy Settings	Select this check box to use the default settings of the Proxy Server specified in Internet Explorer.
Use Proxy Server	Select this check box to specify the required IP address and port number of the Proxy Server in your local network.
Need authentication	Select this check box to specify Proxy Server access credentials in the **Login** and **Password** boxes.
Defaults	Click this button to apply the default settings of the Proxy Server specified in Internet Explorer.

2.6 Status Bar

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

Element	Function
●●●	ACD/I-Lab indicators. For more information, refer to the technical documentation on ACD/I-Lab.
I-Lab Login	Allows you to login to ACD/I-Lab.
-$877.50	Shows your current I-Lab balance.
NONAME01.SK2	Displays the name of the current document (also shown on the title bar).

Element	Function
Modified	Shows the status of the document: either modified or not.
◀▯	Displays the previous page in the current document (if any).
Page 1/1	Shows the number of the current page/number of pages in the document. Clicking this button displays the list of all the pages.
▯▶	Displays the next page in the current document (if any).
Fragments: 3 / Sel. Fragments: 2	In the Structure mode, shows the number of fragments in the workspace or the number of selected fragments.
C_8H_{10}	In the Structure mode, 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). Note that if the **Composition** property is selected (see below), this box displays the percent ratio between drawn atoms of elements: C(88.82%) H(11.18%)
d^{20} : 0.868±0.06 g/cm^3	In the Structure mode, shows the currently selected property calculated for the drawn structure.
Composition	In the Structure mode, displays a menu of different properties of the structure currently displayed. Select one of the properties and the information is provided in the special box on the status bar (see above). Note that this button is labeled with the name of the property currently displayed in the **Properties** box. When a different property is selected, the button label changes accordingly.
Grad: 1.2491 CANCEL	In the Structure mode, during the 3D optimization, shows the progress of the optimization and allows you to cancel it (for more information, refer to Section 3.12.4).

2.7 Structure and Draw Modes

When ACD/ChemSketch starts up, you will find many menu commands and toolbar buttons appear dimmed (inactive). They will be made available as soon as you draw a structure.

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

Structure Draw

In the Structure mode, you can draw 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 ACD/ChemSketch working modes, refer to the chapters that follow.

3. Structure Mode

3.1 Objectives

This chapter acquaints you with:

- The general capabilities of the Structure mode
- The Structure mode interface at a glance
- A detailed description of each command, tool, and interface part available in the Structure mode

To switch to the Structure mode, on the General toolbar, click **Structure** 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 either the elemental composition or the formula and formula weight of the drawn structure(s) or chemical property of the 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. You can 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 by using the integrated ACD/Dictionary (included in the commercial version only). 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.
- Retrieve NMR and Mass reference data from the expanded Periodic Table of Elements.
- Check the most favorable tautomeric forms of the drawn structure and automatically correct the structure by using the integrated **Tautomeric Forms** function on the Structure toolbar.
- Convert 2D structures into their 3D counterparts and view, measure, and handle them in virtual 3D.
- Produce a cleaned-up version of a structure.
- Draw chemical reactions and label reaction arrows to simplify editing of specific experimental conditions. Associate atoms in reactant to product schemes with atom-atom mapping.
- Save or load structures to or from a file on the disk, export or import structures to or from MDL molfiles, cut and paste structures to other Windows applications, by using the **File** menu commands.

3.3 Screen

Below, you can see the screen with the Structure mode enabled. The names and positions of the toolbars and the other elements to be used throughout this manual are introduced.

This table gives the short description of each interface element designated in the above picture:

Interface Element	Function
Title bar	This bar 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).
Menu bar	This bar contains a series of words. Each word links to a list ('menu') of related commands for working in the ChemSketch window in the Structure mode (for a detailed description of each menu and the commands it contains, refer to Sections 3.9–3.19).
General toolbar	This toolbar includes tools that are present in both Structure and Draw modes and will help you with tasks relevant to both modes such as: saving, opening 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).

Interface Element	Function
ChemBasic toolbar	This toolbar includes additional tools that extend the functionality of ACD/ChemSketch. Note that the ChemBasic toolbar is present in both Structure and Draw modes if you have the Goodies tools previously installed (for more information, refer to Appendix C).
Structure toolbar	This toolbar is only present in the Structure mode. It contains tools for drawing and manipulating chemical structures (for more information, refer to Section 3.6).
Atoms toolbar	This toolbar contains buttons representing atoms, as well as tools for changing atom properties (for more information, refer to Section 3.7).
References toolbar	This toolbar contains the Table of Radicals and various buttons representing ready-made radicals you take from the table. You can also access ACD/Dictionary (— ***Commercial version only!***) from this toolbar. For more information, refer to Section 3.8.
Workspace	The workspace is the current ChemSketch page 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).
Status bar	This bar contains information that may be useful for the current moment: name of the opened .SK2 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.
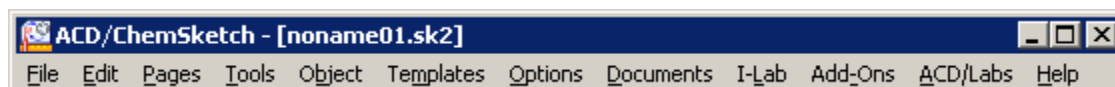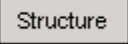
For detailed information on the commands that are available from the menus of the ChemSketch window in the Structure mode, refer to Sections 3.9–3.19.

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/redoing actions, cutting/copying/pasting, and zooming. Most of the buttons on this toolbar are shortcuts of the menu commands; the other buttons are tools that have no corresponding menu command.

The table below gives the short description of all of the buttons available on the General toolbar:

Button	Function	Menu Command
Structure	Switches to the Structure mode.	No corresponding menu command.
Draw	Switches to the Draw mode (for more information on this mode, refer to Section 4).	No corresponding menu command.
You can also press SPACEBAR to switch between the Structure and Draw modes.		

Button	Function	Menu Command
	Adds a new empty document (see Section 3.9.1).	New command (File menu).
	Adds a new empty page at the end of the current document (see Section 3.11.1).	New command (Pages menu).
	Displays the **Open** dialog box where you can specify the name and location of an .SK2 file to be open (see Section 3.9.2).	Open command (File menu)
	Saves the currently open document. When you are saving your work for the first time, the **Save Document As** dialog box prompts you to specify the file name and location (see Sections 3.9.4–3.9.5).	Save or Save As command (File menu)
	Displays the **Print** dialog box where you can specify the required settings for printing the current document (see Section 3.9.12).	Print command (File menu)
	Displays the **Export** dialog box where you can specify the name and location of an Adobe PDF file to which the current document is to be exported (see Section 3.9.7)	Export command (File menu)
	Cancels the last action (see Section 3.10.1).	Undo command (Edit menu)
	Reverts the last canceled action (see Section 3.10.2).	Redo command (Edit menu)
	Enables the **Delete** tool that allows you to delete specific objects in the workspace (see Section 3.5.1).	No corresponding menu command.
	Removes the selected object from the workspace and places it to the Clipboard (see Section 3.10.3).	Cut command (Edit menu)
	Copies the selected object to the Clipboard (see Section 3.10.4).	Copy command (Edit menu)
	Allows you to insert the contents of the Clipboard into the workspace (see Section 3.10.5).	Paste > Default command (Edit menu)
	Enables the **Zoom In** tool that allows you to get a close-up view of objects (see Section 3.5.2).	No corresponding menu command.
	Reduces the display of the objects according to the pre-defined factor (see Section 3.5.3).	No corresponding menu command.
100%	Allows you to control the image scale (see Section 3.5.4).	No corresponding menu command.
	Sets the workspace display to 100% (see Section 3.5.4).	No corresponding menu command.
	Displays the current page to the full width and height in the workspace (see Section 3.5.4).	No corresponding menu command.
	Fits all of the objects on the current ChemSketch page into the workspace (see Section 3.5.4).	No corresponding menu command.
	Fits the selected objects into the workspace (see Section 3.5.4).	No corresponding menu command.

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/Rotate/Resize** tool (Structure mode).

Button	Function	Menu Command
	Displays the **Template Window** dialog box that contains both the built-in and user-defined templates to simplify drawing structures (see Section 3.13.1).	Template command (Templates menu)
	Displays the **Search for Structure** dialog box that allows you to find the required structures in the specified files without opening them (see Section 3.12.25) —*Commercial version only!*.	Search for Structure command (Tools menu)
	Generates the name for the selected structure or structures (see Section 3.12.16).	Generate > Name for Structure command (Tools menu)
	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)
	Runs ACD/3D Viewer (see Section 3.5.5).	No corresponding menu command.
	Closes the active document (see Section 3.9.3).	Close command (File menu).

> **Note** Toolbars of most 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

This button enables the **Delete** tool allowing you to remove objects in the workspace. Note that this tool works differently in the Structure and Draw modes.

Structure mode

In this mode, you can delete both whole chemical structures or graphical objects and the structural fragments or single atoms or bonds.

> **Note** To be able to select and delete the objects created in the Draw mode, as well as reaction pluses and arrows, in the **Preferences** dialog box (**Structure** tab), select the **Select Graphics** check box.

To delete an atom or bond:

• Click **Delete** to enable the corresponding tool, and then click an atom or bond you want to delete.
  The **Delete** tool removes the pointed atom and the adjacent bonds. It never leaves single atoms in the workspace. However, you can retain parts of a structure; hold down CTRL and click a bound atom (for example, the central atom in isobutene). Only the atom you click disappears–all other atoms are retained.
  The **Delete** tool erases the pointed bond. If a single atom is left after the deletion process, it is also automatically removed. However, you can retain all single atoms 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 squares 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 CTRL while selecting them, then release CTRL, point to any of the selection nodes so that they become black, and click.

To delete whole structure(s):

1. With the **Delete** tool active drag over the structure(s) you want to delete so that the selection squares appear.

2. Point to any of selection nodes so that they become black and click.

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

Draw mode

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

To delete an object:

1. Click **Delete** to enable the corresponding tool. Note that the cursor, in this case, becomes an arrow labeled **Del** .

2. Point to the object you want delete so that the contour 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 squares appear.

2. Point to any selected object so that the contours 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 aforementioned regulations.

3.5.2 Zoom Buttons

You can zoom the required part of the workspace using the **Zoom In** and **Zoom Selection** buttons on the General toolbar.

The **Zoom In** button allows you to magnify the workspace. Click this button to enlarge the display of objects from their current magnification up to the next preset scale (see the zoom control box list) and center them on the screen.

The **Zoom Selection** tool allows you magnify the selected part of the workspace. When you click the button, the 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 display.

To restore the fragment to the previous view, use the **Zoom Out** tool.

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

3.5.3 Zoom Out Button
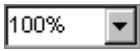
This button enables the **Zoom Out** tool allowing you to reduce the display of the objects from their current magnification to a pre-defined factor every time you click this button.

To magnify an object, on the General toolbar, click **Zoom In** or **Zoom Selection** .

To magnify the screen to specific dimensions, use the **Full Page** , **Page Width** , or **Fit All** tools (for more information, refer to the next section).

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

3.5.4 Zoom Box and Image Scaling Buttons

This box controls the image scale. Choose the percentage of decrease or increase from the drop-down list.

> **Important** This function re-scales the display of the objects on the screen, but does not affect the actual size of the objects. To re-size objects, use 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:

Option	Description	Button
Full Page	Displays the current page to the full width and height in the workspace.	
Page Width	Displays the current page to the full width in the workspace.	
Fit Selected	Fits the selected objects into the workspace.	
Fit All	Fits all of the objects on the current ChemSketch page into the workspace.	
Magnification scale	Select one of the magnification values: 25%, 50%, 75%, 100%, 150%, 200% and 400% to enlarge or reduce the display.	

> **Tip** You can also manually type the percentage value in the box. The minimum available value is 10; the maximum magnification is 500. To input your own value, just click in the box, type the value, and then press ENTER.

3.5.5 3D Viewer Button

This button starts 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

In the Structure mode, below the General toolbar, the Structure toolbar containing buttons for drawing chemical structures is displayed.

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

Button	Description
	Allows you to select and move objects over the workspace (see Section 3.6.1).
	Allows you to select, move, and rotate objects on the workspace (see Section 3.6.2).
	Allows you to rotate the selected structure or structural fragment in 3D (see Section 3.6.3).
	Switches between two modes of selection: lasso and rectangular box (see Section 3.6.4).
	Allows you to draw bonds (see Section 3.6.5).
	Allows you to draw bonds in a continuous mode (see Section 3.6.6).
	Allows you to draw chains (see Section 3.6.7).
	Allows you to draw stereo bonds facing towards the viewer (see Section 3.6.8).
	Allows you to draw stereo bonds facing away from the viewer (see Section 3.6.9).
	Allows you to draw various coordinating bonds (see Section 3.6.10).
	Allows you to draw bonds of some special types (see Section 3.6.11).
	Allows you to draw delocalized bonds (see Section 3.6.12).
	Allows you to draw Markush bonds (see Section 3.6.13).
	Allows you to draw reaction pluses (see Section 3.6.14).
	Allows you to draw reaction arrows. Clicking the white triangle on the button displays more arrow tools (see Section 3.6.15).

Button	Description
	Allows you to label reaction arrows (see Section 3.6.16).
	Allows you to automatically calculate synthesis data for each reaction components (see Section 3.6.17).
a→a	Allows you to map a drawn reaction either manually or automatically (see Section 3.6.18).
[ ]ₙ	Allows you to draw polymers (see Section 3.6.19).
	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).
	Allows you to rotate a chemical structure so that a chosen bond becomes horizontal (see Section 3.6.21).
	Allows you to rotate a chemical structure so that a chosen bond becomes vertical (see Section 3.6.22).
	Allows you to flip a chemical structure or selected fragment on the axis of a chosen bond (see Section 3.6.23).
	Rotates the selected chemical structure on its horizontal axis, giving its mirror reflection (see Section 3.6.24).
	Rotates the selected chemical structure on its vertical axis, giving its mirror reflection (see Section 3.6.25).
	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).
	Redraws and resizes the selected chemical structures to standardize all of the bond lengths and angles (see Section 3.12.2).
	Checks and generates the most reasonable tautomeric forms of drawn organic structures (see Section 3.12.3).
	Creates a 3D model of a 2D chemical structure (see Section 3.12.4).
	Calculates boiling point (BP), vapor pressure (VP), enthalpy of vaporization, and flash point for the selected structure (see Section 3.12.5).
	Calculates and displays monoisotopic mass for several fragments of a structure (see Section 3.12.6).
σ_R	Calculates electronic constants—σ of different types (e.g., inductive, resonance, meta, para etc.) for substituents (see Section 3.6.27).

Note The toolbars of each ACD/Labs program can be customized using the toolbar shortcut menu (for more information, refer to Section 2.2.1).

3.6.1 Select/Move Button

This button enables the **Select/Move** tool allowing you to select and move atoms, bonds, fragments, structures, and graphical objects.

You can quickly switch from the Select/Move mode to the:

- Draw Normal mode ( ) by pressing **ESC**

- Select/Rotate/Resize mode ( ) by right-clicking in the workspace

> **Tip** To be able to select and move objects created in the Draw mode, as well as reaction pluses and arrows, make sure that the **Select Graphics** check box is selected in the **Preferences** dialog box (**Structure** tab). 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 objects (note that the **Select/Move** tool must be active):

To Select	Do This
Atom or bond	Click any atom or bond on the required structure.
Fragment or structure	Drag over the required fragment or structure (you can previously set either **Lasso** or **Rectangular** selection mode; refer to Section 3.6.4).
Multiple structures, fragments	Drag over the required fragments or structures holding down SHIFT (you can previously set either **Lasso** or **Rectangular** selection mode; refer to Section 3.6.4).
Entire structure	Click an empty space in the drawing area adjacent to, but not touching, the structure you wish to select.
All the structures in the workspace	Click an empty space in the drawing area away from any drawn structure until all the structures are selected and marked with hollow squares. Clicking again will deselect all of the structures.
Objects drawn in the Draw mode	Click the object once.
All the objects drawn in the Structure and Draw modes	Press CTRL+A.

Table 2. The table below summarizes the actions you can perform to move objects (note that the **Select/Move** tool must be active :

To Move	Do This
Selected object without snap on grid	If **Snap On Grid** is not selected on the **Options** menu (refer to Section 3.14.3), point to the object so that the contour appears around it (for graphics) or so that the hollow selection squares become black (for structures) and drag. If **Snap On Grid** is selected, hold down SHIFT+CTRL while moving.
Selected object leaving its copy behind	Point to the object so that the contour appears around it (for graphics) or so that the hollow selection squares become black (for structures), press CTRL and hold it down while dragging.
Selected object fixing the object's coordinates along one of the axis	To move the selected object exactly along the X (Y) axis without changing the coordinates along the Y (X) axis, hold down SHIFT while moving.
Selected object snapping on grid	If **Snap On Grid** is not selected on the **Options** menu, hold down SHIFT+CTRL while moving. If **Snap On Grid** is selected, simply drag the object.

> **Note** If the **Informative Cursor** check box in the **Preferences** dialog box (**General** tab) is selected, the new object's coordinates (relative to its original location) are displayed near the cursor.

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

3.6.2 Select/Rotate/Resize Button

This button ![button] enables the **Select/Rotate/Resize** tool allowing you to 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 size of the object display, use the zooming tools (refer to Sections 3.5.2–3.5.4).

> **Note** To be able to manipulate objects created in the Draw mode, as well as reaction pluses and arrows, make sure that the **Select Graphics** check box is selected in the **Preferences** dialog box (**Structure** tab). 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 3. The table below summarizes the actions you can perform to rotate objects:

To Rotate	Do This
Unselected object	Drag the object by any of its elements (the object will be rotated around its center).
Selected object around its center	Point to the object so that the cursor changes to ![cursor] and drag (the object will be rotated around its center). Prior to rotating make sure that the object's action center is located correctly. To view the action center on an object, in the **Preferences** dialog box (**Structure** tab), under **Show**, select **Action Center**.
Selected object around the specified point	1. In the **Preferences** dialog box (**Structure** tab), under **Show**, select **Action Center**. 2. Define the center of rotation either by dragging the action center ![icon] to the required location or by clicking the required location holding down CTRL (action center is placed there automatically in this case). 3. Point to the object so that the cursor changes to ![cursor] and drag.
Selected object in 15 degree increments	Drag the object holding down SHIFT—the selected object will be rotated at the required angle multiple of 15° around its action center.

> **Note** To view the angle of rotation displayed by the cursor, in the **Preferences** dialog box (**General** tab), select the **Informative Cursor** check box.

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

To Resize	Do This
Selected object relative to one of its sides or corners	1. In the **Preferences** dialog box (**Structure** tab), under **Show**, clear **Action Center**. 2. Point to the required selection handle so that the cursor changes to a two-way arrow (![arrow] , ![arrow] , ![arrow] , or ![arrow]), 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	Do This
Selected object relative to the specified point	1. In the **Preferences** dialog box (**Structure** tab), 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 holding down CTRL. 3. Point to the required selection handle so that the cursor changes to a two-way 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.
Selected object relative to its center	Hold down CTRL when dragging a selection handle as described above.
Selected object at certain percent	Hold down SHIFT when dragging a **side** selection handle as described above—the selected object will be resized by percent value multiple of 5.
Selected object so that the height and width change independently	Hold down SHIFT when dragging a **corner** selection handle as described above.

> **Note** To view the percentage of resizing displayed by the cursor, in the **Preferences** dialog box (**General** tab), select the **Informative Cursor** check box.

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

3.6.3 3D Rotation Button

This button 🪐 enables the **3D Rotation** tool allowing you to rotate structures or selected fragments in three dimensions. Click **3D Rotation** 🪐 and point to any bond or atom so that it is surrounded with a rectangle and drag.

Note that the direction of rotation of the front atoms in the 3D-optimized structure 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.

> **Tip** You can designate any bond as the axis of 3D-rotation by clicking it while holding down CTRL. The bond will be marked with red. To cancel this, click the bond once again while holding down CTRL.

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

These buttons 🔍 / 🔲 control the mode used for selecting structures. There are two selection modes. The first mode (🔲) selects objects with the rectangular selection box, while the second mode selects objects with the lasso selector line (🔍). Note that the latter one, the lasso, allows you to select objects in a more specific and precise manner.

To choose between 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

This button enables the **Draw Normal** tool allowing you to draw chemical bonds in the normal mode where, unlike the **Draw Continuous** tool , you can draw new chemical bonds to or from any atom on the screen by clicking the desired atom or dragging from it. Note that the **Draw Normal** tool is automatically on when ChemSketch is loaded.

> **Note**   You can quickly switch between the **Draw Normal** and **Draw Continuous** tools by right-clicking in the workspace.

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

This Action	Does This
Clicking in the workspace.	Draws an atom currently selected on the Atoms toolbar.
Clicking a **separate** atom of the **same** type as the atom selected on the Atom toolbar.	Draws a single bond with the default length.
Clicking a **bound** atom of the **same** type as the atom selected on the Atom toolbar.	Draws a single bond at an angle of 120° to the existing bond.
Clicking a **bound** atom of the **same** type as the selected atom holding down **CTRL**.	Draws a single bond at an angle of 180° to the existing bond.
Clicking an atom of a type **different** from the atom selected on the Atom toolbar.	Changes the atom type to that of the selected one. Note that you can draw a bond having an atom of the selected type at the end with the **Draw Continuous** tool active (for more information, refer to the section that follows).
Clicking a bond.	Switches between possible bond types (single / double / triple).
Dragging.	Draws a single bond at any angle and of any length. If the **Fixed Bond Angle** and **Bond Length** check boxes are selected in the **Preferences** dialog box (**Structure** tab), you can draw bonds of a length multiple to the specified value and at an angle multiple to 15°. If **Snap on Grid** from the **Options** menu is selected, the drawing is constrained by the grid.
Holding down **SHIFT** and **dragging**.	Draws a single bond of a length multiple to the value specified in the **Fixed** area of the **Preferences** dialog box (**Structure** tab) and at an angle multiple to 15°. If the **Fixed Bond Angle** and **Bond Length** check boxes are selected in the **Preferences** dialog box (**Structure** tab), you will draw bonds at any angle and of any length.
Holding down **SHIFT+CTRL** and **dragging**.	Draws a single bond according to the grid. If **Snap on Grid** from the **Options** menu is selected, the drawing is not constrained by the grid.
Right-clicking an empty space.	Switches to the **Draw Continuous** tool .

3.6.6 Draw Continuous Button

This button ![icon] enables the **Draw Continuous** tool allowing you to draw chemical bonds in a continuous mode where, unlike the **Draw Normal** tool ![icon], new chemical bonds can only be drawn from one specific atom which is selected (placed into the black square). If none of atoms is selected, click any atom to select it or click an empty workspace to insert a new atom. Note that only one atom can be selected at a time on the screen.

> **Note** You can switch between the **Draw Normal** and **Draw Continuous** tools by right-clicking in the workspace.

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

This Action	Does This
Clicking in the workspace.	Draws an atom currently selected on the Atoms toolbar and highlights it.
Clicking an existing atom of the **same** type as the atom selected on the Atom toolbar.	Highlights the atom.
Repetitive clicking the same atom.	Draws a single bond with the default length connected to the atom of the same type.
Repetitive clicking any other atom.	Connects the two atoms.
Repetitive clicking in the workspace.	Draws atoms of the same type connected with single bonds.
Clicking an atom of a type **different** from the atom selected on the Atom toolbar.	Highlights the existing atom.
Clicking this highlighted atom for the *second* time.	Draws a single bond of a default length from the highlighted atom and places the atom of the selected type at the end of this bond.
Clicking any other atom for the *second* time..	Connects the two atoms with a single bond.
Repetitive clicking in the workspace.	Draws atoms of the type selected on the Atoms toolbar and connects them with single bonds.
Double-clicking a bound atom.	Draws a single bond connecting an atom of the selected type at an angle of 120° to the existing bond.
Holding down **CTRL** and **double-clicking** a bound atom.	Draws a single bond connecting an atom of the selected type at an angle of 180° to the existing bond.
Clicking a bond.	Switches between possible bond types (single / double / triple).
Dragging.	Draws a single bond at any angle and of any length. If the **Fixed Bond Angle** and **Bond Length** check boxes are selected in the **Preferences** dialog box (**Structure** tab), you can draw bonds of a length multiple to the specified value and at an angle multiple to 15°. If **Snap on Grid** from the **Options** menu is selected, the drawing is constrained by the grid.
Holding down **SHIFT** and **dragging**.	Draws a single bond of a length multiple to the value specified in the **Fixed** area of the **Preferences** dialog box (**Structure** tab) and at an angle multiple to 15°. If the **Fixed Bond Angle** and **Bond Length** are selected in the **Preferences** dialog box (**Structure** tab), you will draw bonds at any angle and of any length.

This Action	Does This
Holding down **SHIFT+CTRL** and **dragging**.	Draws a single bond according to the grid. If **Snap on Grid** from the **Options** menu is selected, the drawing is not constrained by the grid.
Right-clicking an empty space.	Switches to the **Draw Normal** tool ⬚.

3.6.7 Draw Chains Button

This button ⬚ enables the **Draw Chains** tool allowing you to draw atom chains. To draw a long atomic 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, in the **Preferences** dialog box (**General** tab), select the **Informative Cursor** check box.

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

This Action	Does This
Clicking in the empty space.	Draws an atom currently selected on the Atoms toolbar.
Clicking a single atom of the same type as the atom selected on the Atoms toolbar.	Draws a bond with the default length.
Clicking a bound atom of the same type as the selected atom.	Draws a bond at an angle of 120° to the existing bond.
Holding down **CTRL** and **clicking** a bound atom of the same type as the selected atom.	Draws a bond at an angle of 180° to the existing bond.
Clicking an atom of a type different from that of the selected atom.	Changes atom type to that of the selected one.
Clicking a bond.	Switches between possible bond types (single / double / triple).
Dragging	Draws 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 in the **Preferences** dialog box (**Structure** tab), you can draw bonds of a length multiple to the specified value and at an angle multiple to 15°. If **Snap on Grid** from the **Options** menu is selected, the drawing is constrained by the grid.
Holding down **CTRL** and **dragging**	Draws 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 in the **Preferences** dialog box (**Structure** tab), you can draw bonds of a length multiple to the specified value and at an angle multiple to 15°. If **Snap on Grid** from the **Options** menu is selected, the drawing is constrained by the grid.
Holding down **SHIFT** and **dragging**.	Draws a chain at a fixed length and fixed angle of 15°. If the **Fixed Bond Angle** and **Bond Length** check boxes are selected in the **Preferences** dialog box (**Structure** tab), you will draw bonds at any angle and of any length.

This Action	Does This
Holding down SHIFT+CTRL and dragging	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.
Right-clicking an empty space.	Switches to the **Draw Normal** tool .

3.6.8 Up Stereo Bonds Button

This button enables the **Up Stereo Bonds** tool allowing you to draw stereo bonds facing towards the viewer in a 3-dimensional representation of the drawn structure. When this tool is active, new chemical bonds can be drawn in the same way as with the **Draw Normal** tool (for more information, refer to Section 3.6.5). The differences between these tools are:

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

To change a normal bond, down stereo bond (a bond that is away from the viewer), or coordinating bond to a stereo bond that is facing towards the viewer, activate this tool and click the bond.

You can switch between the **Up Stereo Bonds** and the **Down Stereo Bonds** tools by right-clicking in the workspace.

3.6.9 Down Stereo Bonds Button

This button enables the **Down Stereo Bonds** tool allowing you to draw stereo bonds that are facing from the viewer in a 3-dimensional representation of the drawn structure. When this tool is active, new chemical bonds can be drawn in the same way as with the **Draw Normal** tool, but there are some differences between these tools:

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

To change a normal bond, an up stereo bond, or a coordinating bond to a bond that is facing away from the viewer, activate this tool, and then click the bond.

You can switch between the **Down Stereo Bonds** and the **Up Stereo Bonds** tools by right-clicking in the workspace.

3.6.10 Coordinating Bonds Buttons

These buttons enable the set of tools allowing you to draw coordinating (non-covalent) bonds. To display all of the possible types, click the right bottom triangle on the button.

The following types of coordinating bond buttons are available:
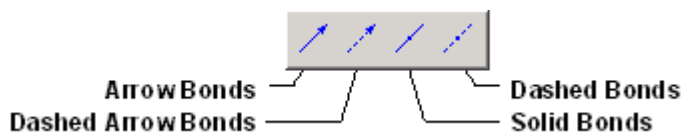
With one of the coordinating bonds active, new chemical bonds are drawn in the same way as with the **Draw Normal** tool, but there are some differences between these tools:

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

To change a normal bond, an up stereo bond or a down stereo bond to a coordinating bond, activate the required **Coordinating Bonds** tool by clicking the corresponding button, and then click the bond.

> **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.

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

3.6.11 Special Bonds Buttons

These buttons enable the set of tools allowing you to draw various types of bonds. To display all of the possible types, click the right bottom triangle on the button.

The following types are available:
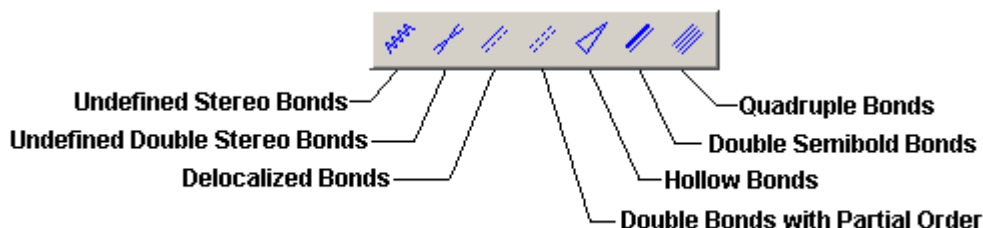
With one of the special bonds active, new chemical bonds are drawn in the same way as with the **Draw Normal** tool. The differences between these tools are:

* When a new bond is placed between two atoms or generated 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 a normal bond, an up stereo bond, or a down stereo bond to a special bond, activate the required **Special Bonds** tool by clicking the corresponding button, and then click the bond.

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

This set of buttons ⌃ ⌃ allows you to draw solid or dotted curves indicating the delocalized chemical bonds.

Clicking the right bottom triangle of the button displays the following buttons:

⌃ **Solid Delocalization Curve**

⌃ **Dotted Delocalization Curve**

To insert the delocalization curve, draw the structure or select the fragment (or structure) for which you want to insert a curve, and then click any of these buttons. The curve will automatically appear.

> **Important** To apply this option, 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 option, the action center is displayed which is not visible while printing. You can place it wherever you need by dragging it.

It is possible to drag an atom or bond in the selected fragment in the workspace. Any new bond can be drawn from the center by clicking and dragging.

If necessary, you can change an atom in the selected fragment, the curve is not deleted at that. 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 type in the structure.

The charges or radical particles present in the structure will be moved on the action center after you click any of these ⌃ ⌃ buttons. Note that you can also set charge or radical particle on the action center manually; on the Atoms toolbar, click the required **Charge/Radical Particles** button (refer to Section 3.7.6), and then click the action center.

3.6.13 Markush Bond Buttons

These buttons enable the tools that allow you to attach a Markush bond to a structure or a selected structural fragment. The resulting structure is generic (it represents a group of corresponding structures) where the Markush bond denotes the variability in position of a substituent within the structure.

Clicking the right bottom triangle of the button displays the following buttons:

Markush Bond

Markush Bond with Shadow

Added or Removed Fragment

Added or Removed Fragment with Shadow
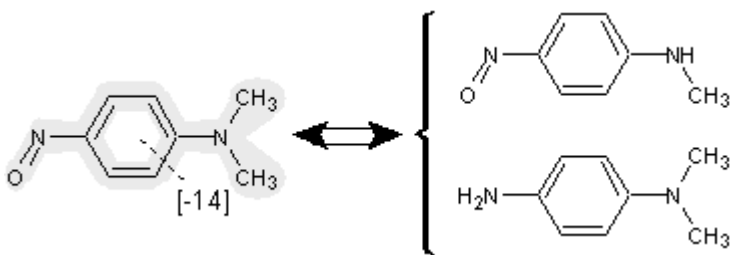
To attach a Markush bond, click the required atom on the Atoms toolbar or select the one in the Periodic Table (this atom will be at the end of the Markush bond), select the required structure in the workspace (if there is more than one structure drawn), and click any of the **Markush Bond** buttons. If nothing is selected in the structure and you click the button, a warning message will appear asking if you wish to attach the Markush bond to the whole structure.
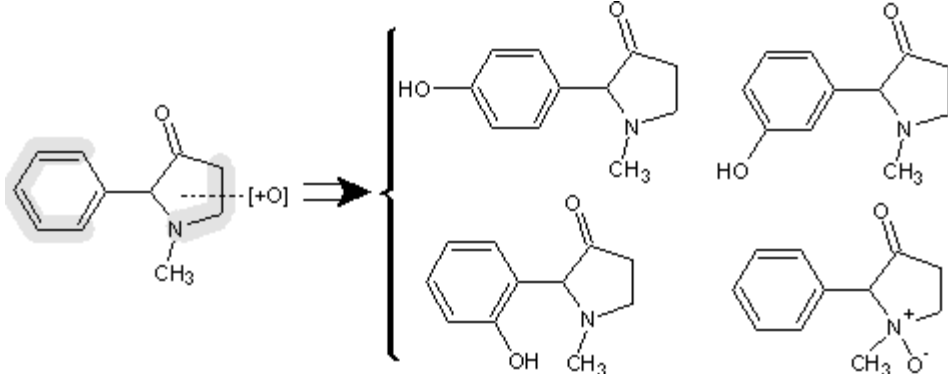
To visibly display the atoms a Markush bond refers to, use the **Markush Bond with Shadow** tool.

To draw the structures with the attached mass or formula difference values, instead of the added

or removed structural fragments themselves, click **Added or Removed Fragment** or **Added**

or Removed Fragment with Shadow . The **Define Markush Mass Difference** dialog box appears.

This dialog box contains the following options:

Option	Function
Additional / Subtraction	In this area, select whether the difference value will be marked as added (**Additional**) or removed (**Subtraction**).
Mass	Select this option to attach the mass difference value as a Markush label.
	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 Subtraction and Mass options, and then, in the adjacent box, type 14. The following created structure represents the oxygen atom removal from the nitroso group or monodemethylation:
	Both structures have formula weight 14 units less than initial N,N-dimethyl-4-nitrosoaniline.

Option	Function
Fragment	Allows you to attach the formula difference as a Markush label; select this option, and then, in the adjacent box, type a needed formula difference.
	For example, the following Markush structure with the added oxygen fragment describes at least three hydroxylation products and amine oxide at the same time:

> **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

This button ➕ enables the **Reaction Plus** tool allowing you to draw a reaction plus in the Structure mode.

Select this 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 3.14.1.3.
>
> 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

These buttons enable the set of tools allowing you to draw various reaction arrows in the Structure mode. Click the bottom right triangle of the button to expand it into more **Reaction Arrow** buttons:

To insert an arrow, choose the required **Arrow** tool and click in the workspace to place an arrow of a standard length or drag to draw an arrow of desired length. Clicking the arrow for the second time will delete it.

> **Note** You can change the color and style of reaction arrows in the **Preferences** dialog box (**Reaction** tab). For more information on this dialog box, 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 in the **Preferences** dialog box (**Structure** tab).

You can switch between the available reaction arrow tools by right-clicking in the workspace.

3.6.16 Reaction Arrow Labeling Button
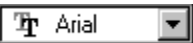
This button enables the tool allowing you to insert labels that specify the appropriate reaction conditions.

To insert reaction conditions, with this tool enabled, click the reaction arrow. In the **Edit Reaction Conditions** dialog box that appears, type your own comment or click several buttons from the conditions set on the right side of the dialog box. Click **OK**.
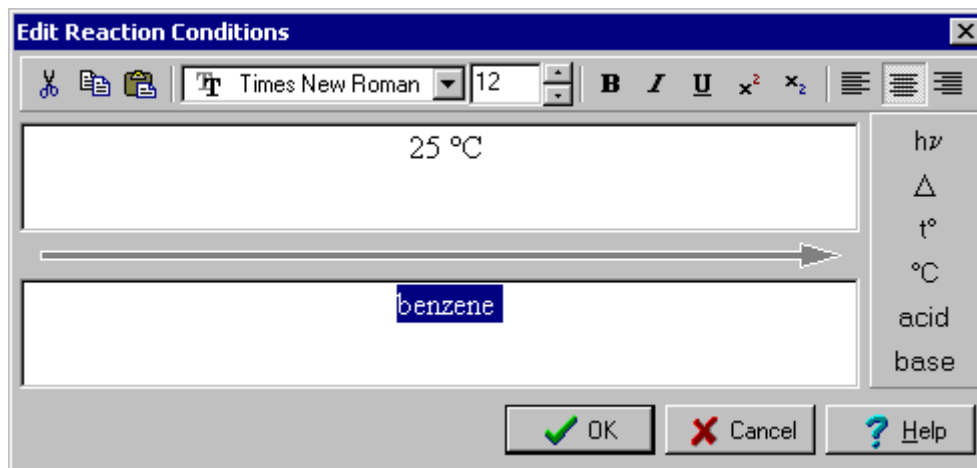
This dialog box contains the following options:

Option	Function
(cut icon)	Cuts the selected text and places it to the Clipboard.
(copy icon)	Copies the selection to the Clipboard.
(paste icon)	Inserts the contents of the Clipboard at the insertion point or, if a string is selected, replaces it.
Tr Arial ▼	In this box, you can specify the appropriate font style.
10 ▲▼	In this box, you can specify the size of the font.
B	Formats the selected text with bold. Click this button again to cancel formatting with bold.
I	Formats the selected text with italic. Click this button again to cancel formatting with italic.
U	Underlines the selected text. Click it again to cancel underlining.
x^2	Formats the selected text with superscript. The superscript button is automatically enabled when you type a formula in any of the panes. For example, atom charge is automatically turned into superscript.
x_2	Formats the selected text with subscript. The subscript button is automatically enabled when you type a formula in any of the panes. For example, the atom number index is turned into subscript.
(align left icon)	Aligns the text left.
(center icon)	Centers the text.
(align right icon)	Aligns the text right.
Upper Pane	In this pane, you can specify the conditions for the reaction; the conditions will be placed above the reaction arrow.
Lower Pane	Click in the lower pane and then type or select conditions specific for the reaction to place them below the reaction arrow.
hv	Inserts the **hv** symbol (lighting) at the insertion point or, if a string is selected, replaces it.
Δ	Inserts the Δ symbol (heat applied) at the insertion point or, if a string is selected, replaces it.
t°	Inserts the **°t** symbol at the insertion point or, if a string is selected, replaces it.
°C	Inserts the **°C** symbol at the insertion point or, if a string is selected, replaces it.
acid	Inserts **acid** as your reaction condition at the insertion point or, if a string is selected, replaces it.
base	Inserts **base** as your reaction condition at the insertion point or, if a string is selected, replaces it.
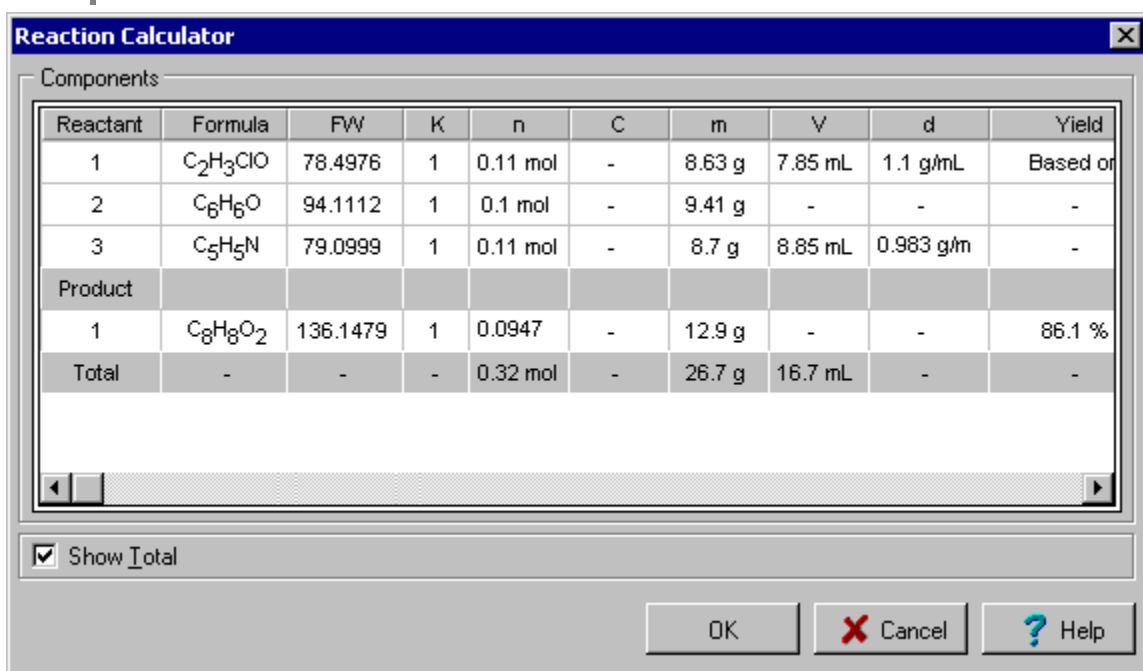
> **Note**   If you export the Reaction Conditions set through the **Reaction Arrow Labeling** tool into an .RXN file, the previously specified conditions will be lost.

3.6.17 Reaction Calculator Button

This button ⊞ enables the tool allowing you to automatically calculate synthesis data for each reaction components.

To calculate data, with this tool enabled, click the reaction arrow; the **Reaction Calculator** dialog box appears. It contains the **Components** table with the following columns: molecular formula and formula weight (these columns are filled in automatically), stoichiometric coefficient (**K**), quantity (**n**), concentration (**C**), mass (**m**), volume (**V**), density (**d**), as well as yield of products (**Yield**).

> **Note** To provide the automatic calculation of the 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.

Reaction Calculator

Components

Reactant	Formula	FW	K	n	C	m	V	d	Yield
1	C_2H_3ClO	78.4976	1	0.11 mol	-	8.63 g	7.85 mL	1.1 g/mL	Based on
2	C_6H_6O	94.1112	1	0.1 mol	-	9.41 g	-	-	-
3	C_5H_5N	79.0999	1	0.11 mol	-	8.7 g	8.85 mL	0.983 g/m	-
Product									
1	$C_8H_8O_2$	136.1479	1	0.0947	-	12.9 g	-	-	86.1 %
Total	-	-	-	0.32 mol	-	26.7 g	16.7 mL	-	-

☑ Show **T**otal

OK   ✗ Cancel   ? Help

To edit the reaction 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. (To provide the calculation of mass and quantity, you need to type the density value.)

Note that the **Yield** is always relative and its calculation is based on the component with the lowest amount. To calculate yield, double-click the cell corresponding to the product under **m** (mass) and type the proper value, then press ENTER. You will see that the yield is calculated and the "*Based on*" notation appears under **Yield** in 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 filled in **Components** table in the ChemSketch page.

3.6.18 Atom-Atom Map Button

This button [a→a] enables the **Mapping** tool allowing you to map a drawn reaction either manually or automatically. As you click the button, the **Map Tools** panel appears and the mapping mode is enabled.

The **Map Tools** panel contains the following buttons:

Button	Function
Manual Mapping	Enables the Manual Mapping mode (note that this mode is set by default). Now, you can assign atoms of the reactant to the corresponding atoms of the product manually by pointing to a chosen atom and dragging to its counterpart.
Select Reaction	Works just like the **Select/Move** tool (for more information on this tool, refer to Section 3.6.1) except for not allowing you to move objects.
Auto Mapping	Maps 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.
Delete Mapping	Cancels the mapping of all 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.

It is possible to perform both automatic and manual mapping on 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, in the **Manual Mapping Color** box of the **Preferences** dialog box (**Reaction** tab), set the appropriate color. For automatic mapping, in the **Auto/Manual Numbering Color** box of the **Preferences** dialog box (**Structure** tab), set the appropriate color.

Whenever you close the **Map Tools** panel, you quit the mapping mode and atom numbers are no longer visible.

> **Tip** You can export the mapped reactions to ACD/ChemFolder (as a REACCS.RXN file) or to ISIS/Draw (as an ISIS/Sketch .SKC files).

3.6.19 Polymers Button

This button [ ]n enables the **Polymers** tool allowing you to turn a structure or fragment into a polymer. Clicking this button displays the **Polymer** panel where you can specify the required options.

This panel contains the following options:

Option	Description
Index	In this box, specify the index for your polymer (any number or letter). As you click **Apply**, it will appear at the lower right corner of the right bracket.
Connectivity	In this box, select the way the units are connected in your polymer: ***head-to-tail***, ***head-to-head***, or ***either/unknown***. The default setting is head-to-tail so the upper right corner of the right bracket is empty, while head-to-head, or either/unknown types produce 'hh' and 'eu' respectively.
Style	Select the way your polymer will look: in brackets [ ], in parenthesis ( ), or in braces { }.
Apply	Applies the defined parameters to the selected polymer.

To draw a polymer, follow the steps:

1. Draw one or more structures you want to turn into a polymer.

2. On the Structure toolbar, click **Polymers** [ ]ₙ and, on the **Polymer** panel that appears, specify the required settings.

3. Select the area you want to turn into a polymer either by clicking or by dragging. Note that you can turn the entire structure or part of two structures into one polymer only by dragging.

As soon as the area is selected, the polymer appears in the workspace.

> **Tip** When drawing polymers, for your convenience only, hold down CTRL when clicking/dragging with the **Draw Normal**, **Draw Continuous**, or **Draw Chains** tools. Each of these combinations allows you to draw a bond at an angle of 180° to the existing bond rather than 120° (created when CTRL is not pressed); thus creating more customary-looking structures. For more information on how to use these combinations, refer to Sections 3.6.5, 3.6.6, and 3.6.7.
>
> To create end-open structures, replace the end atoms in a drawn polymer with empty atoms using the **Pseudo Atom** tool (refer to Section 3.7.5).

3.6.20 Change Position Button

This button ⊗ enables the **Change Position** tool allowing you to change the arrangement of a double bond or the display position of a hydrogen atom, to control the bonds intersection point, and to specify the connection point of an atom label.

You can do the following with this tool:

- Each additional click on a **double bond** with this tool active switches between the three double bond types shown below:
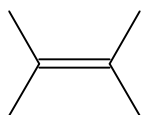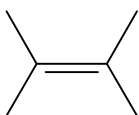
| Symmetric | Asymmetric 1 | Asymmetric 2 |
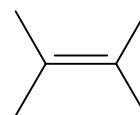
- Each additional click on an **atom** with this tool active switches between various position of the hydrogen. Hydrogen(s) can be displayed around the base symbol in four positions:

H_2N N H_2 NH_2
                  H_2 N

       Left   **Bottom**   **Top**   **Right**
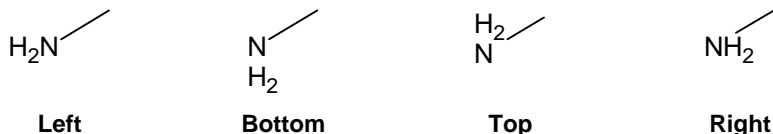
- When the bonds are intersecting, one of them is displayed as a background bond and another as a foreground bond. To bring the background bond to the front, hold down SHIFT and click it with the **Change Position** tool active.

- Atom labels 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 on the label. To change the connection symbol on the label, hold down SHIFT and click repeatedly the atom label with the **Change Position** tool active. The label will shift and, as the needed atom becomes a connection point, stop clicking. If you click the label without holding down SHIFT, the program will connect the bond to either the first or last symbol on the label.

3.6.21 Set Bond Horizontally Button

This button* ▽ enables the **Set Bond Horizontally** tool allowing you to rotate a chemical structure so that the desired bond becomes horizontal.

To place the required bond horizontally, make this tool active and then click this bond. As the selected bond becomes horizontal, the whole structure is rotated accordingly. Each additional click on the same bond rotates the structure by 180°.

3.6.22 Set Bond Vertically Button

This button* ↑ enables the **Set Bond Vertically** tool allowing you to rotate a chemical structure so that the desired bond is displayed vertically.

To place the required bond horizontally, make this tool active and then click this bond. As the selected bond becomes vertical, the entire structure is rotated accordingly. Each additional click on the same bond rotates the structure by 180°.

3.6.23 Flip on Bond Button

This button* 🖉 enables the **Flip on Bond** tool allowing you to rotate a chemical structure or selected fragment on the axis of a chosen bond.

To flip a structure on one of its bonds, make this tool active and then click the required bond. You can also flip a structure on the selected fragment.

> **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.

---

* Before using this command, verify whether the whole chemical structure is selected or only a part of it. When only parts of a structure have been selected, this command may, by changing the angles between bonds, cause unwanted changes in the chemical structure. If this happens, click **Undo** ↩ .

3.6.24 Flip Top to Bottom Button

This button* enables the **Flip Top to Bottom** tool allowing you to turn chemical structure(s) about the horizontal axis.

Select the structure you want to rotate and click this button. If no structure or fragments are selected on the current page, clicking this button flips all of the drawn structures as a single object. Flipping structures having optical center produces enantiomers.

> **Note**   If the **Select Graphics** check box is selected in the **Preferences** dialog box (**Structure** tab), 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

This button* enables the **Flip Left to Right** tool allowing you to turn chemical structure(s) about the vertical axis.

Select the structure you want to rotate and click this button. If no structure or fragments are selected on the current page, clicking this button flips all of the drawn structures as a single object. Note that flipping structures having optical center produces enantiomers.

> **Note**   If the **Select Graphics** check box is selected in the **Preferences** dialog box (**Structure** tab), 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

This button enables the **Instant Template** tool allowing you to 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. Click **Instant Template** .

3. Point to the structure or selected structural element and click. The shadow of the selected structure or element becomes attached to the cursor.

> **Note**   If you are going to use the template for attaching it to the already drawn structure, make sure that you click the most suitable atom or bond when creating a 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 shadow by pressing TAB.

---

* Before using this command, verify whether the whole chemical structure is selected or only a part of it. When only parts of a structure have been selected, this command may, by changing the angles between bonds, cause unwanted changes in the chemical structure. If this happens, click **Undo** .

4. Move it to the desired location in the workspace and click to paste.

> **Note** When inserting the template taken by an atom, if you click the atom of the drawn structure while holding down SHIFT, the atom of the template will replace the atom you click (the template will be attached without a bond).

You can use the 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 this template again, you should create it again.

3.6.27 Calculate Parameters of Substituent Button

This button $\boxed{\sigma_R}$ can be used to calculate electronic substituent constants—σ of different types (e.g., inductive, resonance, *meta*-, *para*-, *etc.*) for your substituents. It also calculates some steric constants (MV and MR, i.e., the molar volume and molar refractivity) and a hydrophobic constant (the π constant of Hansch) for a fragment of your compound. This option is useful for correlation of different properties which depend on characteristics of substituents attached to a constant reaction center.

This module must be purchased in addition to ACD/ChemSketch. For more details on sigma calculation, refer to *ACD/Sigma Pro 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 includes 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 of each tool:

Button	Function
	Displays the Periodic Table of Elements (see Section 3.13.5).
A / **Any**	Enables the **Query Atom** / **Query Bond** tools that allow you to specify search queries for performing a substructure search (see Sections 3.7.1–3.7.2).
C **H** **N**	Use these buttons to draw the corresponding atoms in the workspace (see Section 3.7.3).
abc	Enables the **Edit Atom Label** tool that allows you to insert and change atom labels (see Section 3.7.4).
/ **R**	This tool allows you to insert pseudo atoms or radical designation labels (see Section 3.7.5).
+	Enables the **Charge/Radical Particles** tool that allows you to change the atom's charge and to draw radical particles (see Section 3.7.6).
ᴵAᴼₙ	This tool allows you to change the chemical properties of an atom (see Section 3.7.7).
#	Enables the **Manual Numbering** tool that allows you to number atoms on the drawn structure(s) manually (see Section 3.7.8).

> **Note** To customize the toolbar contents, right-click it to display the context menu (for more information, refer to Section 2.2.1).

3.7.1 Query Atom Buttons

These buttons enable the set of tools allowing you to specify the query atoms when performing a substructure search. Click the bottom right triangle of the button to expand it into more buttons:

Button	Description
A **Any Atom**	The marked atom may be any atom but hydrogen.
Q **Any Heteroatom**	The marked atom may be any atom except carbon or hydrogen.
H0 **Any Atom without Hydrogen**	No hydrogens can be attached to this atom.
L **Atom from List**	Creates a list of atoms to be allowed.
NL **Atom Not in List**	Creates a list of atoms to be excluded.

To specify query atoms for a substructure search, click the required button from a set of tools, and then click the atom of the structure which you want to be replaced with the query atom.

> **Note** When you mark query atoms in a structure, you can use the structure only as a search query. You cannot store this structure in a database except for the ACD/SpecDB database, version 6.0 or later.

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

3.7.2 Query Bond Buttons

These buttons enable the set of tools allowing you to specify the query bonds when performing a substructure search. Click the bottom right triangle of the button to expand it into more buttons:

Button	Description
Any **Any Bond**	The marked bond can be any type of bond (single, double, triple, or aromatic).
Ar **Aromatic Bond**	The marked bond can only be aromatic.
S/D **Single or Double Bond**	The marked bond can only be single or double bonds (but not aromatic or triple).
Rn **Ring Bond**	The marked bond must be part of a ring (cancels chain).
Ch **Chain Bond**	The marked bond must be part of a chain (cancels ring).

To specify query bonds for a substructure search, click the required button from a set of tools, and then click the bond in the structure which you want to be replaced with the query one.

> **Note** When you mark query bonds in a structure you can only use the structure as a search query. You cannot store such a structure in a database except for ACD/SpecDB database, version 6.0 or later.

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

3.7.3 Atom Buttons

These buttons can be used to quickly insert atoms of required 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 to choose it.

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

- Click in the empty space to insert the chosen atom.

- With the **Draw Normal** ![tool] tool active, click any atom in the drawing area to replace it with the chosen atom.

- With the **Draw Continuous** ![tool] tool active, click an atom twice to sprout a new single bond with the chosen atom.

- With the **Draw Chains** ![tool] tool active, draw atom chains with the chosen atom as the binding point.

For more information on these tools, refer to Sections 3.6.5–3.6.7 correspondingly.

If the required element is not listed on the Atoms toolbar, click ![icon] to display the **Periodic Table of Elements** dialog box where you can choose the required element (note that the selected element will be placed on the Atoms toolbar as a new button).

To remove user-selected atoms from the Atoms toolbar, double-click the toolbar.

For non-metals, the inserted atom appears in its lowest valence as a hydride derivative, whereas for metals, the inserted atom appears in its lowest oxidation state as an ion. You can change the atomic charge and/or oxidation state of an atom by using the **Increment(+) Charge** ![+] or

Decrement (–) Charge ![–] buttons (for more information, refer to Section 3.7.6) 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** ![icon] (for more information, refer to Section 3.7.7).

2BStructure Mode

3.7.4 Edit Atom Label Button
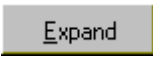
This button abc enables the **Edit Atom Label** tool allowing you to insert a label in an empty space or to replace any atom in a structure with a group abbreviation or a label which then can be expanded. To insert a label, click the **Edit Atom Label** tool and then click the needed atom or empty space. 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 then change the connection point of the label by using the **Change Position** tool (for more information, refer to Section 3.6.20).

This dialog box contains the following options:

Option	Description
Format area	The tools in this area allow you to format an input label.
Label box	In this box, type the label you want to insert or choose the corresponding one from the list below. Note that the three last used labels are saved in the list and are displayed with red at the top (they cannot be deleted). To save your label or delete the existing ones, use the buttons to the right. To show only standard or user labels, use the options in the **List** area.
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)**.
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.

Option	Description
Insert	Replaces the selected atom with the specified label or inserts the label in the empty workspace of the ChemSketch page.
Expand	Expands the specified label (represents it as a structure). The atom label can be expanded only if it was entered in capitals. Also, only group abbreviations 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 (ACD10 for version 10.0). 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

These buttons $\boxed{\mathcal{P}}$ / $\boxed{R}$ enable the set of tools allowing you to replace atoms with radical labels or pseudo atoms. If you click the bottom right triangle of the button, it will be expanded into more buttons:
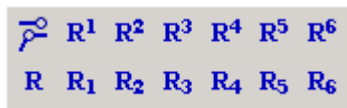
Click the required button to make active the corresponding tool, and then click the atom to replace it with the label or pseudo atom.

> **Tip** To insert pseudo atoms, you can also double-click a highlighted atom to display the corresponding **Properties** panel; in the **Value** box of the **Atom** tab, select '*Empty*', and then click **Apply**.

Use the **Pseudo Atom** $\boxed{\mathcal{P}}$ tool to create open-ended polymers and bent bonds. Bent bonds are ignored in calculations (treated as standard bonds).

3.7.6 Charge/Radical Particles Buttons

These buttons enable the set of tools allowing you to change atom's charge or to make radicals from the existing atoms. Click the bottom right triangle of the button to expand it into more buttons:

To apply any of these tools, click the required button and then the atom you want to modify.

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

These buttons [+] / [−] enable tools allowing you to change the charge of a chosen non-metal atom or both the charge and oxidation state of a chosen metal. To apply the required charge, click the button and then click the desired atom in the workspace. The atomic charge and/or oxidation state increases in increments or decreases in decrements according to the valid oxidation states for metals or the valid valences for non-metals.

> **Note**   These two options 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** [icon] button.

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

3.7.6.2 Radical Particles Buttons

The **Radical** button [•] enables the tool allowing you to create radicals. The subsequent clicking the atom with this tool active changes the atom to:

- Monoradical, for example $CH_3^{\bullet}$
- Singlet biradical, for example $CH_2\colon$
- Triplet biradical, for example $^{\bullet}CH_2^{\bullet}$

The **Positive Radical Ion** button [+•] enables the tool allowing you to create positive radical ions, for example $CH_4^{+\bullet}$. To do this, click any atom with this tool active.

The **Negative Radical Ion** button [−•] enables the tool allowing you to create negative radical ions, for example $CH_4^{-\bullet}$. To do this, click any atom with this tool active.

> **Note**   Right-clicking in the workspace with any of the aforementioned tools active switches between them.

3.7.7 Atom Chemical Properties Button

This button ⬛ enables the **Atom Chemical Properties** tool allowing you to set new properties for a drawn atom. To edit the properties of the required atom, click the atom with this tool active. In the **Atomic Properties** dialog box that appears, specify the required settings.

This dialog box contains the following options:

Option	Description
Valence	In this box, specify the valence value. It should be a number from 0 to 8.
Charge	In this box, specify the charge value. Note that you can also define radical particles.
Isotope	In this box, specify the isotopic mass value.
Numbering	In this box, specify a numerical or textual string to be used as a numbering for the selected atom.
Keep non-typical visibilities	This check box is available in case you have manually set some of the visible characteristics (e.g., presence of valence or isotope) through the **Properties** panel (refer to Section 3.12.1). To keep the previously set visible characteristics, select this check box.
Mode	Saves the properties you have specified in this box and adds them as a new **Atom Chemical 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 ''properties'' 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

Clicking this button ⊞ displays the **Manual Numbering** dialog box where you can number atoms in the workspace manually.
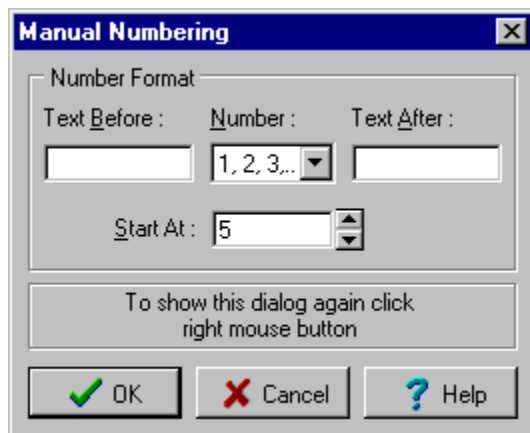
This dialog box contains the following options:

Option	Description
Text Before	In this box, type the text to be inserted before each inserted number.
Number	From the list of available number styles, choose the required one.
Text After	In this box, type the text to be inserted after each inserted number.
Start At	In this box, specify the value from which the numbering should be started.
OK	Closes the dialog box and enables the **Manual Numbering** tool.
Cancel	Closes the dialog box and disables the **Manual Numbering** tool.

> **Tip** You can also display this dialog box by right-clicking in the workspace with the **Manual Numbering** tool active.

To set atom numbering, follow the steps:

1. On the Atoms toolbar, click **Manual Numbering** ⊞. This will display the **Manual Numbering** dialog box.

2. Specify the type of numbering, if required, enter the text before and after a number and specify the starting number.

3. Click **OK**. Note that cursor becomes ⊞. Then click the desired atom on the workspace. It will be assigned the specified starting number. Subsequent clicking of other atoms in the workspace will continue numbering.

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

To edit atom numbering, click the required atom with this tool active and specify new settings in the dialog box.

> **Note** You can specify the color of atom numbers in the **Auto/Manual Numbering** box of the **Preferences** dialog box (**Structure** tab). For more information on this dialog box, refer to Section 3.14.1.2.
> You can change the style (font size, color, etc.) of the atom number labels on 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.

This toolbar contains the following buttons:

Button	Function
![icon] —*Commercial version only!*	Displays ACD/Dictionary. For more information, refer to Section 3.13.6.
![icon]	Displays the Table of Radicals containing the most frequently needed radicals for a quick structure drawing. For more information, refer to Section 3.13.4.
Shortcut buttons for radicals	These shortcut buttons appear when you select a radical from the Table of Radicals at least once and can be removed from the toolbar by double-clicking it.

> **Note** To customize the toolbar contents, right-click it to display the shortcut menu. For more information, refer to Section 2.2.1.

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. On the **File** menu, you can see the history of last loaded files. Click the file you want to load again.

3.9.1 New

This command creates a new empty 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 document active, select it from the list on the **Documents** menu.

> **Note** ACD/ChemSketch allows you to have up to ten documents open at once. If you have ten documents open, the **New** command will become inactive until one is closed.

Shortcut:

General toolbar: ![icon]
Keyboard: CTRL+N

3.9.2 Open

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

The following formats are supported:

- ChemSketch 2.0 Document (.SK2)
- All supported Chemical Files (.MOL, .SKC, .RXN, .CHM, .CDX, .MST, .RPT)
- MDL molfiles (.MOL)
- ISIS/Sketch (.SKC)[1]
- MDL RXNfiles (.RXN)
- ChemSketch 1.0 (.MST, .RPT)
- CS ChemDraw (.CHM, .CDX)[2]
- Windows Metafiles (.WMF)[3]

As soon as you open the document, its name is displayed in the left corner of 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 inactive until at least one document 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, you are prompted to confirm whether to save changes or not. If this is the last open document, ChemSketch automatically creates a "noname" one. As you close a document, ChemSketch prompts you to save your work if you've not already done so.

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

Shortcut:

Keyboard: CTRL+W

General toolbar

3.9.4 Save

This command allows you to save the active document as an .SK2 file. If you are saving your work for the first time, the **Save Document As** dialog box appears prompting you to specify the

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[1] 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.
[2] You can import objects from the CS ChemDraw files of any versions later than 3.0.
[3] While importing Windows Metafiles, note that the bitmaps from the imported file will not be placed into ACD/ChemSketch.

file name and location. If your work has been saved before, the existing file parameters are used (the name and location of the file are displayed on the title bar).

> **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
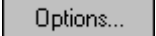
3.9.5 Save As

This command allows you to display the **Save Document As** dialog box where you can specify a new name, location, and format for the currently open ChemSketch document.

The following formats are supported:

‣   ChemSketch 2.0 Document (SK2)

‣   MDL Molfiles (.MOL)

‣   ISIS/Sketch (.SKC)

‣   MDL RXNfiles (.RXN)

‣   CS ChemDraw (.CHM, .CDX)

‣   MDL Extended Molfiles (.MOL)

‣   CML files (.CML)

‣   Adobe Acrobat (.PDF) – you can also use the **Export to PDF** button on the General toolbar.

‣   Windows Metafiles (.WMF)

‣   Windows Bitmaps (.BMP, .DIB)

‣   Paintbrush (.PCX)

‣   TIFF Bitmaps (TIF)

‣   GIF Bitmaps (.GIF)

‣   Portable Network Graphics (.PNG)

If you are saving data to TIFF Bitmap or Portable Network Graphics format, you can define some options in the **TIFF Export Options** and **Potable Network Graphics Export Options** dialog boxes (refer to Section 3.9.5.1), which can be displayed by clicking **Options** .

> **Tip** If you want to save a file with the same name and to where it currently resides, 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 TIFF Export Options / Portable Network Graphics Export Options Dialog Box

This dialog box allows you to set the required image resolution for the active file you are working with.

This dialog box appears when you choose **TIFF Bitmap (.TIF) / Portable Network Graphics (*PNG)** in the **Set as type** drop-down list and click **Options** `Options...` in the **Save Document As**/**Export** dialog box.

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:
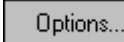
  Keyboard: SHIFT+ F12

3.9.7 Export

This command allows you to export the contents of the active document into one of the supported external formats. This command displays the **Export** dialog box where you can specify the format, name, and location of a file to be exported.

The following formats are supported:

‣ MDL Molfiles (.MOL)

‣ ISIS/Sketch (.SKC)

‣ MDL RXNfiles (.RXN)

‣ CS ChemDraw (.CHM, .CDX)

‣ MDL Extended Molfiles (.MOL)

‣ CML files (.CML)

‣ Adobe Acrobat (.PDF) – you can also use the **Export to PDF** button on the General toolbar.

‣ Windows Metafiles (.WMF)

‣ Windows Bitmaps (.BMP, .DIB)

‣ Paintbrush (*.PCX)

‣ TIFF Bitmaps (*TIF)

‣ GIF Bitmaps (*GIF)

‣ Portable Network Graphics (*PNG)

If you are exporting data to TIFF Bitmap or Portable Network Graphics format, you can define some options in the **TIFF Export Options** and **Potable Network Graphics Export Options** dialog boxes (refer to Section 3.9.5.1), which can be displayed by clicking **Options** | Options... |.

3.9.8 Import

This command allows you to import objects from one of the supported external formats. It displays the **Import** dialog box where you can specify the name and location of a file you want to import.

The following formats are supported:

- All supported Chemical Files (.MOL, .SKC, .RXN, .CHM, .CDX, .MST, .RPT)
- MDL molfiles (.MOL)
- ISIS/Sketch (.SKC)[4]
- MDL RXNfiles (.RXN)
- ChemSketch 1.0 (.MST, .RPT)
- CS ChemDraw (.CHM, .CDX)[5]
- Windows Metafiles (.WMF)[6]

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 allows you to display the **Run Program** dialog box where you can specify the name and location of a program (.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 details on ACD/ChemBasic and ACD/Forms Manager, refer to the corresponding documentation.

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[4] 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.
[5] You can import objects from the CS ChemDraw files of any versions later than 3.0.
[6] 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 allows you to display the **Page Setup** dialog box where you can specify page settings either for the whole document or for the current page.

It contains the following options:

Option	Description
Size&Orient	On this tab, you can specify the paper format and orientation of the drawing: either landscape or portrait (for more information, refer to Section 3.9.11.1).
Margins	On this tab, you can set margins for the page to be printed (for more information, refer to Section 3.9.11.2).
Poster	On this tab, you can set the number of pages your poster will consist of (if you are going to print a poster). For more information, refer to Section 3.9.11.3.
Apply To	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 current document only (**Current Page**). If there is the only page in the document, this option is not available.
Preview Field	Shows the results of the specified settings.
Set Default	Saves the currently specified paper size, orientation, and margins as default.
Restore Default	Changes the current settings to the last accepted default settings. If no defaults have been recently set, this button has no effect.

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.
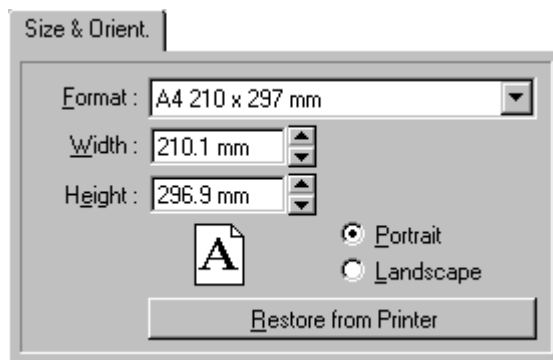
This tab contains the following options:

Option	Description
Format	In this box, specify the paper size available for your printer. As you choose the paper format, the **Width** and **Height** boxes display the corresponding values. If you choose *Custom Size*, you can specify your own format.
Width	This box displays the width* of the currently set paper format. As you start typing your own value, the **Format** box displays *Custom Size*.
Height	This box displays the height* of the currently set paper format. As you start typing your own value, the **Format** box displays *Custom Size*.
Portrait	Choosing this option will allow you 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.
Landscape	Choosing this option will allow you 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.
Restore From Printer	Changes the current page configuration (paper size and orientation only) to the printer settings.

3.9.11.2 Page Setup Dialog Box: Margins Tab

On this tab, you can set margins for the page to be printed. This function does not constrain your drawing it only draws a line showing the margins.
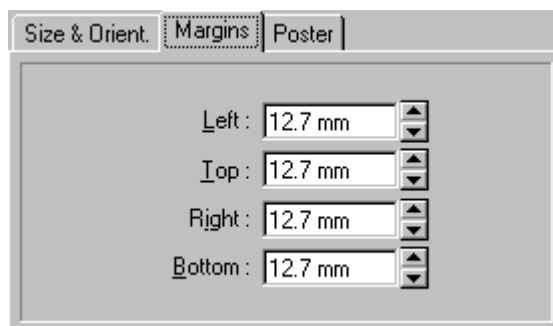
This tab contains the following options:

Option	Description
Left **Top** **Right** **Bottom**	In these boxes, specify the amount of space* between the left/top/right/bottom edge of the paper and the corresponding margin of the page.

To display the margins on the ChemSketch page(s), select the **Page Margins** check box in the **Preferences** dialog box (**General** tab). For more information on this dialog box, refer to Section 3.14.1.1.

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* 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.

3.9.11.3 Page Setup Dialog Box: Poster Tab

If you are going to print the poster, on this tab, you can set the number of pages your poster will consist of.

This tab contains the following options:

Option	Description
Width Calculation	In this box, you can specify the number of standard pages (the size page dimensions is specified on the **Size & Orientation** tab) for the width of the poster. Note that the maximal number of pages for the width is 5. The calculated poster size will be displayed in the **Virtual Page Size** area.*
Height Calculation	In this box, specify the number of standard pages (the standard page size is specified on the **Size & Orientation** tab) for the height of the poster. Note that the maximal number of pages for the height is 4. The calculated poster size will be displayed in the **Virtual Page Size** area.*
Virtual Page Size	This area displays the calculated virtual size of a poster.

3.9.12 Print

This command allows you to print the active document using the current printer defaults. 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.

As you choose this command, the **Print** dialog box is displayed allowing you to specify which pages of the document you want to print, the number of printed copies, and the printer to use.

> **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 in white, the structures will not be visible on the printout if you cancel background color.

Shortcuts:

Keyboard: CTRL+P

General toolbar:

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* 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.

3.9.13 Print Preview

This command allows you to display each page as it will look on the printout. You can view multiple pages at a time, and magnify or reduce the size of the page on the screen.

The view that appears incorporates the following buttons:

Button	Function
🖨	Prints the active document.
🔍⊕	Zooms in to get a close-up view of the document. You can zoom in using the button in the Print Preview mode or by pressing the PLUS SIGN (+) on the numeric keypad.
🔍⊖	Zooms out to see more of the page (multiple pages) at a reduced size. You can zoom out using the button in the Print Preview mode or by pressing the MINUS (–) on the numeric keypad.
☐	Displays only one page. You can also display one page by pressing the ASTERISK (*) on the numeric keypad.
◀☐	Displays the first page in the current document.
◀☐	Displays the previous page in the current document (if any).
☐▶	Displays the next page in the current document (if any).
☐▶|	Displays the last page in the current document (if any).
☒	Quits print preview and returns to the previous view of the document.

3.9.14 Properties

This command displays the **Document Properties** dialog box, which allows you to set the properties (descriptive title, subject, author name, organization, and other user information in the file) for the active ACD/ChemSketch document which will help you to track the data.

This dialog box contains the following options:

Option	Description
Title	Type the title you want to use when searching for the file.
Subject	Type 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.
Author	By default, this box contains your system login. To change the author, delete the existing name, and then type a new one.
Organization	Type your company name.
Comments	Enter the comments for your file.
Set As Default Properties	If you select this check box, the information specified in this dialog box will be automatically inserted into the properties for newly created documents.
Statistics	Displays the dates when the document was created and modified, and the file size.

3.9.15 Send > As Is / As PDF

Use these commands to send the current document by e-mail either as an .SK2 or .PDF file.

When you choose the appropriate command, your default 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 mail client is set as the default.

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 sending.

If you have opened a new document and have not saved it yet, ACD/ChemSketch will give it a default name (*noname 01*, *02*...).

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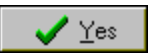
3.9.16 File Associations

This command displays the **File Associations** dialog box where you can assign certain file formats to ACD/ChemSketch.
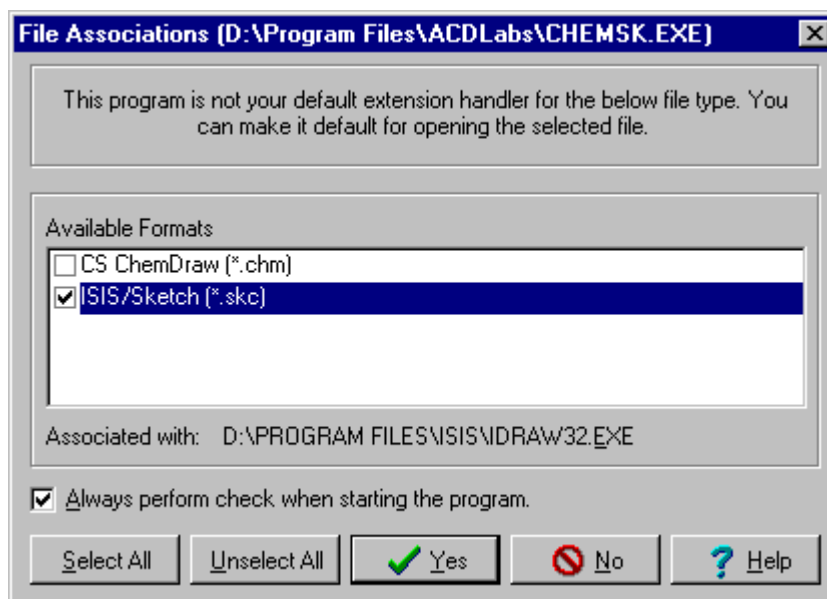
The following options are available in this dialog box:

Option	Description
Available Formats	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 shows the application to which the currently highlighted format is linked.
Always perform check when starting the program	If this check box is selected, each time ACD/ChemSketch is started it will verify whether there are formats supported by your version that are not associated with it yet. If there are any, this dialog box will appear at the startup.

Option	Description
Select All	Click this button to select all of the file formats in the **Available Formats** box.
Unselect All	Click this button to cancel the selection of all the file formats in the **Available Formats** box.
✓ Yes	Click this button to close the dialog box applying the specified settings.
🚫 No	Click this button to close the dialog box without applying association.

If the file formats have been already associated with the program, the corresponding message will be displayed.

If you open the **File Associations** dialog box under Windows NT but have no rights to change file associations, a warning message appears. Contact your system administrator to resolve this matter.

> **Note**   You can change file association through Windows Explorer: hold down SHIFT and right-click the required file, then, from the shortcut menu that appears, choose **Open With**, and specify the application that should be used to open the file.

3.9.17 Exit

Use this command to close ACD/ChemSketch. Note that 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 **Close All**.

> **Note**   ChemSketch will prompt you to save your work unless you have just done so.

Shortcuts:

Keyboard: ALT+X
Mouse: double-click the application control menu button (in the upper left corner of the window).

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 edit the sketch contents, i.e., to cut, copy, paste, and undo actions.

3.10.1 Undo

This command allows you to cancel the last actions performed. This command can be used up to 50 times in sequence so that you can restore almost any previous stage of your work. To reverse the effect of the **Undo** command, from the **Edit** menu, choose **Redo**.

Shortcuts:

Keyboard: ALT+BACKSPACE

General toolbar:

3.10.2 Redo

This command allows you to cancel 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 edits made to your work. To reverse the effect of the **Redo** command, from the **Edit** menu, choose **Undo**.

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

Shortcuts:

Keyboard: 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 into other Microsoft Windows applications as well as other documents within ACD/ChemSketch, or other parts of the same document.

> **Note**   When pasting structures copied from ACD/ChemSketch to other applications (e.g., Microsoft Excel), the structure may be represented as a set of numbers and figures (as a MDL molfile). To place a picture of the structure, use the **Paste Special** feature in 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 ChemSketch by double-clicking on the picture.

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 into other Microsoft Windows applications as well as other documents within ACD/ChemSketch, or other parts of the same document.

> **Note** When pasting structures copied from ACD/ChemSketch to other applications (e.g., Microsoft Excel), the structure may be represented as a set of numbers and figures (as a MDL molfile). To place a picture of the structure, use the **Paste Special** feature in 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 ChemSketch by double-clicking on the picture.

Shortcuts:

Keyboard: CTRL+C

General toolbar:

3.10.5 Paste > Default

This command pastes the last object added to the Clipboard into the document. Once this command is selected, the cursor with the attached shadow of the object from the clipboard appears. Click the desired location to place the object.

> **Note** If the object has been placed onto the Clipboard from an external application (not ACD/ChemSketch), it will be pasted as an embedded object and can be edited in the application it has been taken from. To paste the object in different 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 or 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 allows you to paste objects from the Clipboard in a specific format. As you choose this command, the **Paste Special** dialog box with clipboard formats available for the current contents of the Clipboard appears. Select the needed format and click **OK**. The Clipboard contents appear attached to the cursor. Click in the desired location to paste the object.

To edit the object pasted in this way, double-click it. If the object has not been created in ACD/ChemSketch, but 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 objects will be updated in the ChemSketch window correspondingly.

> **Note** To insert 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**.

3.10.8 Paste > Structure

This command pastes chemical structure(s) from the Clipboard. It is useful for inserting chemical structures that were not created with ACD/ChemSketch (for example, from ISIS/Draw). Unlike the **Paste Special** command, this command places structure(s) created with other applications not as a picture but as chemical structure(s) so that you can edit them in the Structure mode. If the Clipboard does not contain a structure, this command is disabled.

> **Note** The possibilities of the **Paste Structure** function are limited so some structures can be pasted incorrectly.

3.10.9 Paste > Table

This command pastes the Clipboard contents into 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 attached to the cursor. Click the desired location to paste the copied objects.

> **Note** To insert an object created with another application in your ChemSketch document 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 cannot use the **Paste** commands to retrieve the objects erased with **Delete**; however, you can retrieve them 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. For more details on how to select/unselect individual objects in the Structure mode, refer to Sections 3.6.1–3.6.2.

> **Note** If the **Select Graphics** check box is cleared in the **Preferences** dialog box (**Structure** tab), the objects created in the Draw mode are not 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 the 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 dialog box with the list of the supported applications appears.

2. Select an application and click **OK**. The application, if available and properly installed, will be opened.

3. In this application, create, open, or modify a file.

4. Quit the application to return to ACD/ChemSketch. The object is embedded in the left upper corner of 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 that was previously embedded with the **Insert Object** command.

As you select the object and choose this command, the application associated with the object is started. After making the necessary changes, quit the application to return back to ACD/ChemSketch where the object is automatically updated.

> **Note** You will 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 creates a new blank page at the end of the document and makes it active. One document can contain up to 100 pages.

Shortcut:

   General toolbar:

3.11.2 Insert

This command creates a new blank page before the current page and makes it active.

Shortcut:

   Keyboard: SHIFT+F3

3.11.3 Change Order

This command allows you to rearrange pages in your document. It displays the **Change Order of Pages** dialog box where you can see the current page number and specify a new number for the page by typing or using the arrows. The other pages are reordered accordingly. Note that this command is disabled if you have opened one-page document.

3.11.4 Delete

This command removes the current page and its contents from the current 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, once deleted, the page can be recovered with the **Undo** command until you quit ChemSketch.

Shortcut:

   Keyboard: SHIFT+F4

3.11.5 Rename

This command allows you to rename the current page of a document. Clicking this command displays the **Rename Page** dialog box. 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 **Page List**:
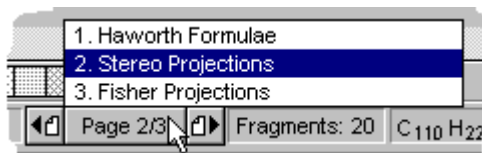
> **Note**   You can use the **Number/Annotate Page** goody for page annotation. For more information, refer to Appendix C.

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 displays the Header and Footer toolbar that allows you to create headers/footers for the pages in your document. Headers and footers can consist of text or graphics. As in other applications, a header appears at the top of a page and a footer appears at the bottom.

The toolbar incorporates the following buttons:

Button	Function
Insert AutoText	Inserts common header or footer items in your document. From the drop-down list, choose the item you want to insert into header/footer. The information is placed in tags (unrepresented text of document markup) containing braces and macro elements. The macro elements denote the following: $N—page numbers $S—total page numbers $A—author's name $O—organization name $L—document title $J—document subject $F—file name $P—path with file name $T—time $D—date 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 .HFP file to be loaded into the current document.
	Displays the **Save Document As** dialog box where you can specify the name and location of an .HFP file to which the current footer and header are to be saved.
	Closes the Header and Footer toolbar and applies your settings.

> **Tip** You can use this feature to insert a background picture for your document. When in the Edit Header/Footer mode, draw or insert the picture and place it in the required position on the page. When you leave the editing mode, the picture will become a background for your drawings.

3.11.8 Header and Footer > Load

This command allows you to load the header and footer previously saved to an .HFP file.

3.11.9 Header and Footer > Save

This command allows you to save the header and footer of the current document to an .HFP file, 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.

3.11.10 Header and Footer > Save As

This command allows you to display the **Save Document As** dialog box where you can specify the name and location of an .HFP file 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 allows you to display the **Set Header/Footer Page as Default** dialog box where you can specify an .HFP file whose header and footer are to be used by default, that is, they will automatically be inserted in 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.

To cancel the default header and footer, click **Clear Default**.

3.11.12 Header and Footer > Clear
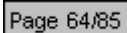
This command removes both the header and footer from the current document.

3.11.13 Header and Footer > Show

This command toggles the display of headers and footers in the document. Note that this command is selected by default.

3.11.14 Previous

This command displays the previous page of the document. Note that this command is disabled if you have opened one-page document.

You can also click **Page List** `Page 64/85` (displays the current page's number and the overall number of pages in the current document) on the status bar to quickly switch to the required page.
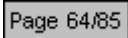
Shortcuts:

   Keyboard: PAGE UP
   Status bar:

3.11.15 Next

This command displays the next page of the document. Note that this command is disabled if you have opened one-page document.

You can also click **Page List** `Page 64/85` (displays the current page's number and the overall number of pages in the current document) on the status bar to quickly switch to the required page.
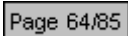
Shortcuts:

    Keyboard: PAGE DOWN
    Status bar: `◁▶`

3.11.16 First

This command displays the first page of the document. Note that this command is disabled if you have opened one-page document.
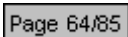
You can also click **Page List** `Page 64/85` (displays the current page's number and the overall number of pages in the current document) on the status bar to quickly switch to the required page.

Shortcut:

    Keyboard: CTRL+HOME

3.11.17 Last

This command displays the last page of the document. Note that this command is disabled if you have opened one-page document.

You can also click **Page List** `Page 64/85` (displays the current page's number and the overall number of pages in the current document) on the status bar 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 containing properties of the currently selected structure(s). You can also open this panel by double-clicking the structure with the **Select/Move** tool 🔍 active. On this panel, you can specify the graphic representation of chemical drawings.
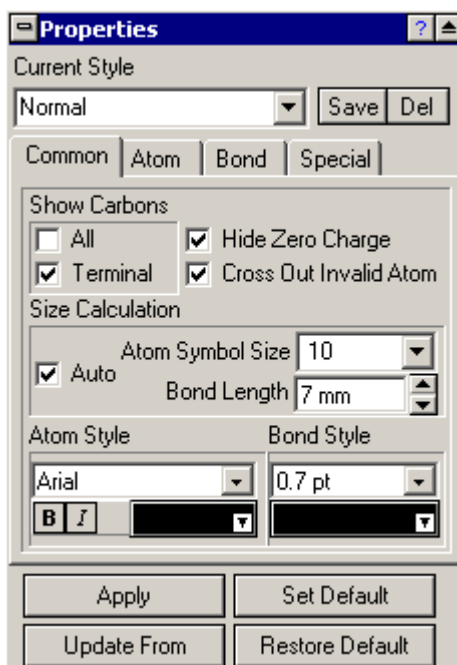
The table below gives the general description of the panel parts:

Option	Description
Normal ▼ Save Del	This set of options allows you to load the style attributes from any of the existing styles, save a user-defined style, and delete any of the user-defined styles. **To load the style**, click the arrow and choose the style from the list. To apply it to the selection, click **Apply** at the bottom of this panel. **To name your own style**, set the required options in the panel, click in this box, type the name of the style, and click **Save**. **To delete the style**, find it in the list and click **Del**.
Common tab	On this tab, you can specify settings common for both atoms and bonds of the selected structure(s). For more information, refer to Section 3.12.1.1.
Atom tab	On this tab, you can set the view options of atoms. For more information, refer to Section 3.12.1.2.
Bond tab	This tab contains options for changing the display of bonds. For more information, refer to Section 3.12.1.3.

Option	Description
Special tab	On this tab, you can specify the style settings for the Markush bond shadow. For more information, refer to Section 3.12.1.4.
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 the newly drawn structures automatically.
Update From	Enables the update feature allowing you to copy style attributes from the drawn structure to the panel. As you click this button, the cursor becomes an arrow labeled **From** **FROM** . Click with it a structure to update its style settings to this panel.
Restore Default	Restores the settings of the current default style on the panel.

Shortcuts:

Keyboard: CTRL+SHIFT+S
Mouse: double-click a fragment or atom

3.12.1.1 Properties Panel: Common Tab

This tab allows you to specify the style settings for the selected structural fragments or structures.
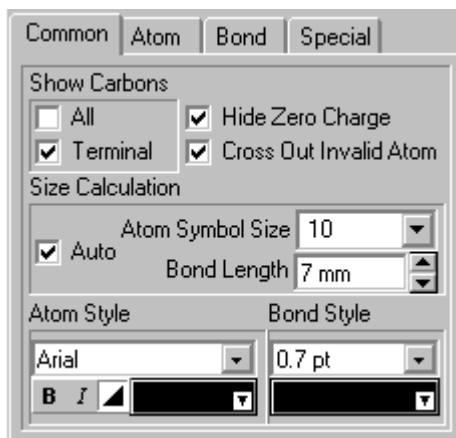
This tab contains the following options:

Option	Description
Show Carbons	The check boxes located in this area control whether all of the carbons or terminal carbons only should be displayed. Select/clear the All or Terminal check boxes.[*] If none of the check boxes is selected, no carbons will be displayed in the selected structure.
Hide Zero Charge	This check box controls whether the zero charges should be displayed.*

---

[*] 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 the state of the current attribute differs for the selected objects), i.e., this attribute will not be changed for the selected objects.

Option	Description
Cross Out Invalid Atom	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**.[*]
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, you can specify the style for atom labels. If the selected atoms are of mixed style, the **Own** button ◢ is enabled.
Bond Style	In this area, you can set the bond thickness** and color.

3.12.1.2 Properties Panel: Atom Tab

On the **Atom** tab, you can specify the style settings for the selected atom labels.
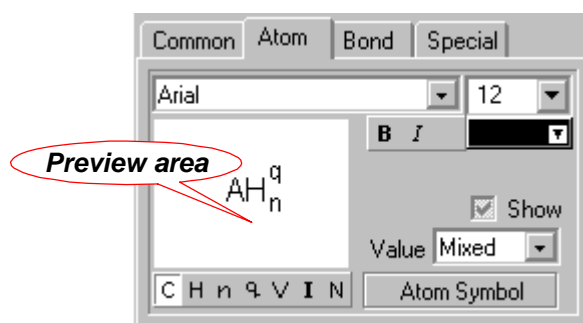
Each label is represented with a set of attributes:

C	atom symbol
H	hydrogen
n	index
q	charge
V	valence
I	isotope
N	numbering

To change the settings for any of them, click the corresponding button below the preview area. To apply the same style settings to several kinds of atom attributes at a time, hold down SHIFT and click the required buttons in the row of attributes.

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

---

[*] 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 the state of the current 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.

The following options are available:

Option	Description
Arial ▾	In this box, you can specify the font style to be applied to the symbol(s) currently selected below the preview area.
8 ▾	In this box, you can specify the font size to be applied to the symbol(s) currently selected below the preview area.
B *I* ◢	Allow you to make the corresponding symbols in the atom labels **bold** */ italic / **bold italic***. If the **Own** button ◢ is enabled, it means the current attribute has mixed formatting in the selection.
▾	In this box, you can specify the color for the symbol(s) currently selected below the preview area.
Show	This check box controls whether the selected attribute should be shown in the structure or not.*
Value	This box is present for atom symbol C, hydrogen H, charge q, valence V, isotope I and numbering N and allows you to set the corresponding value for any of these attributes. For the atom symbol, if you choose **Empty**, no atom symbol will be inserted. For the hydrogen symbol H, in this box, you can specify the position of the hydrogen: auto position, left, right, bottom, or top relative to the basic atom symbol. Note that to make this box appear on the panel you should previously select one atom only.
Y	This box is present for hydrogen index n, charge q, valence V, isotope I and numbering N and allows you to set the Y-coordinate** of the corresponding attribute relative the basic atom symbol.
After H	This check box controls the position of the valence symbol V in the atom label. If you select this check box, the valence symbol will be placed after hydrogen.*
Soft	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 (+) Charge** + or **Decrement (–) Charge** − tools on the Atoms toolbar, the charges are set as 'soft'.*
X	In this box, specify the X value that controls the position of the numbering symbol N relative to the atom label along the X-axis. Note that the coordinates can have a negative value.*

---

* 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 the state of the current 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.

3.12.1.3 Properties Panel: Bond Tab

On the **Bond** tab, you can specify the style settings for the selected bonds.
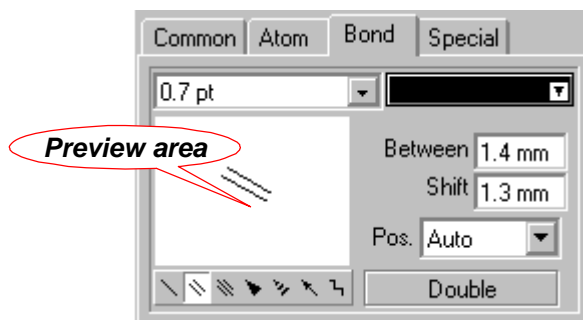
The following types of bonds are available:

	single bond
	double bond
	triple bond
	up stereo
	down stereo
	coordinating bond
	undefined bonds

To change the settings for any of them, click the corresponding button below the preview area. To apply the same style settings to several kinds of bonds at a time, hold down SHIFT and click the required buttons in the row of bond types.

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

The following options are available for bond attributes:

Option	Description
0.7 pt	In this box, you can specify the line thickness* to be used for the corresponding type of bond.
	In this box, you can specify the color for the bond lines of the type currently selected below the preview area.
Between	In this box, you can specify the distance between the lines for double bond and triple bond.
Shift	This box is present for double bond and triple bond. For double bonds, in this box, you can specify the shift (i.e., difference in length) between the lines when the bond is defined as a symmetric. For triple bonds, in this box, you can specify the difference* between the central line length and the length of other two lines in a bond.
Pos.	In this box, you can specify the position of two lines in a double bond relative to each other. You can see the specified position in the preview area.
Width	In this box, you can specify the thickness* of the wider end for up stereo and down stereo bonds, and the width* of sections for undefined bonds

---

* If several objects are selected, these check boxes may have three statuses: **cleared**—does not apply the current option to all the selected objects, **selected—**applies the current option to all the selected objects, and **grayed—**does not change the current option of the selected objects).

Option	Description
Step	In this box, you can specify the step between the sections representing down stereo ⬆ and undefined bonds ⬆.
H. Length **H. Width**	In these boxes, you can specify the length and width of the arrowhead for coordinating bond ⬉.

3.12.1.4 Properties Panel: Special Tab

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

The following options are available:

Option	Description
Show	Controls whether the Markush bond shadow should be shown in the structure or not.
■ **Solid**	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.
▨ **Pattern**	Click this button to shadow the Markush bond using a diagonal strip pattern. You can specify the prototype and color for hatching in the **Color** and **Pattern** boxes to the right.
Mix **Mixed**	The active **Mixed** button indicates that the state of the Markush bond shadow in the selected objects differs and will not be changed.
Color	In this box, you can specify the color to be applied to the selected Markush bond.
Pattern	In this box, select the needed pattern for hatching.

3.12.2 Clean Structure

This command redraws and resizes the selected chemical structure(s) to standardize all of the 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 "cleaned".

The **Clean Structure** function standardizes all of 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, in the **Preferences** dialog box (**Clean** tab), select the required checkboxes (for more information, refer to Section 3.14.1.4).

If the results are not satisfactory, use **Undo** 🔄 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 apply the **Clean Structure** command again.

Shortcuts:

Structure toolbar: 🔴
Keyboard: F9

3.12.3 Check Tautomeric Forms

This command checks and generates the most reasonable tautomeric forms of drawn organic structures.

As soon as the forms are generated, the **Check Tautomeric Forms** dialog box appears with the suggested predominant tautomeric forms displayed.

> **Note**   If the drawn structure is the major tautomeric form itself, selecting this command displays the corresponding message.

This dialog box contains the following options:

Option	Description
Information	Displays the number of tautomeric forms suggested.
Structure	Displays the drawn chemical structure as the dialog box is open. As you click the **Next** `Next >>` and **Previous** `<< Prev.` buttons below, this area displays the suggested tautomeric forms.
`<< Prev.` `Next >>`	Use these buttons to browse through the tautomeric forms.
`Replace`	Replaces the drawn structure with the structure currently displayed in the Structure area.

Shortcuts:

Structure toolbar:
Keyboard: CTRL+SHIFT+T

3.12.3.1 ACD/Tautomers Algorithm

The following information will help you to gain a better understanding of the features of the current algorithm.

The ACD/Tautomers algorithm recognizes and takes into account most of the known types of tautomeric equilibrium such as:

- Aldehydes, ketones, thioaldehydes, thioketones—enoles, thioenoles;

- Imines—enamines;

- Oximes—nitrozocompounds;

- Nitrocompounds—aci-form of nitrocompounds;

- 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 equilibria 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 forms. 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, sulphur, 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-dimensiomal model of a planar (2D) chemical structure. This option can be applied to only one selected structure at a time. While optimization is being carried out, the status bar displays the progress and allows you to cancel at any time. After the 3D optimization is complete, the 3D model is automatically available for 3D rotation if the **Switch to 3D-Rotation Mode** check box in the **Preferences** dialog box (**Structure** tab) is selected (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.

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 (1983)). The modifications involve some simplification and were intended to increase the stability and speed of computation. Note that 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.

If you try to obtain a specific enantiomer for a structure with chiral centers, in the process of optimization, the configuration input may occasionally change to an opposite one. To solve the problem, it is usually enough to draw all four substituents of the chiral atom and use both **Up** 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 answering "No" when you are asked whether to remove hydrogens before starting optimization in the unfolding **3D Structure Optimization** dialog box.

You may wish to perform actual conformational analysis of your structure using a special molecular mechanics or quantum chemistry geometry optimization package. ChemSketch 3D-optimized structure 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 the up and down stereo bonds to define the stereoconfigurations, 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 calculates boiling point (BP), vapor pressure (VP), enthalpy of vaporization, and flash point for the selected structure. Choosing this command opens the **ACD/Boiling Point** dialog box with a graph illustrating the calculated BP or VP.

> **Note**   This module must be purchased in addition to ChemSketch.

For more details on the **Boiling Point** dialog box options, refer to the *ACD/Boiling Point User's Guide.*

Shortcuts:

Structure toolbar:
Keyboard: CTRL+SHIFT+B

3.12.6 MassSpec Scissors

This command calculates and displays monoisotopic mass for several fragments of a structure. Select bond(s) connecting fragments for which you want to calculate monoisotopic mass, and choose this command or click **MassSpec Scissors** . Monoisotopic mass values will appear beneath the all fragments.

> **Note** To calculate nominal mass and average mass values for a structure fragment, select it and then choose the corresponding command from the **Calculate** submenu (**Tools** menu).

If you select three and more adjoining bonds simultaneously, the warning message appears informing you that all of the selected bonds will be broken as a result of this operation, and it looks that a part of a molecular structure or the whole structure has been selected accidentally. Click **Yes** to continue the process anyway or **No** to cancel it.

Shortcut:

Structure toolbar:

3.12.7 Show Aromaticity

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

> **Note** To remove aromatic circles, from the **Tools** menu, choose **Hide Aromaticity**.

Shortcut:

Keyboard: CTRL+SHIFT+A

3.12.8 Hide Aromaticity

This command transforms the delocalized double bonds in aromatic rings into the conjugated double bonds in all of the structures on the current page or in the selected structure(s) or fragment(s).

> **Note** To show aromatic circles, from the **Tools** menu, choose **Show Aromaticity**.

Shortcut:

Keyboard: CTRL+SHIFT+H

3.12.9 Expand Shorthand Formulae

This command expands a label based on the shorthand formula inserted with the help of the **Edit**

Atom Label tool � (for more information, refer to Section 3.7.4). Select the label you want to expand and choose this command. If no structure(s) or fragments are selected, this command affects all of the drawn structures on the current page.

The following symbols are acceptable by this tool:

'~' (tilde)—negative charge;

'+' (plus)—positive charge;

'–' (minus)—single bond (can be omitted);

'=' (equal sign)—double bond;

'%' (percent)—triple bond;

'( )' (brackets)—embrace a group of atoms.

> **Note**   You can find conventions for label expanding in the EXPAND.TXT file. The left column in this file contains notations supported by the **Expand** tool. It is not recommended to modify this file.

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 working area, explicit hydrogens are added to all of the structures drawn on the current page.

To remove explicit hydrogens, from the **Tools** menu, choose **Remove Explicit Hydrogens**.

> **Note**   If you choose to optimize the structure with explicit hydrogens in 3D, you are asked whether to remove explicit hydrogens before 3D optimization. Even if you choose **Yes**, the hydrogens may still appear in the 3D optimized structure if the **Add Hydrogens** option in the **Preferences** dialog box (**Structure** tab) is selected. For more information, refer to Section 3.14.1.2.

Shortcut:

Keyboard: CTRL+SHIFT+Y

3.12.11 Remove Explicit Hydrogens

This command hides explicit hydrogens from the selected fragment or structure. If no structure(s) or fragments are selected, explicit hydrogens will be removed from all of the drawn structures on the current page.

To add explicit hydrogens, from the **Tools** menu, choose **Add Explicit Hydrogens** (for more information, refer to Section 3.12.10).

Shortcut:

Keyboard: CTRL+SHIFT+R

3.12.12 Bring Bond(s) to Front

This command allows you to switch the selected background bond to foreground. Select the bond and choose this command.

If the **Enable Bond Intersections** check box in the **Preferences** dialog box (**Structure** tab) is selected, ACD/ChemSketch automatically breaks the bond behind the new bond that is drawn. The broken bond is considered to be the background bond and the unbroken one is considered to be in the foreground.

Background Bond
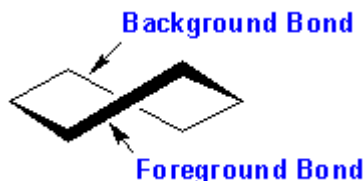
Foreground Bond

> **Tip** You can also bring background bond to front using the **Change Position** ⟨icon⟩ tool (refer to Section 3.6.20).

Shortcut:

   Keyboard: CTRL+F

3.12.13 Send Bond(s) to Back

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

> **Tip** You can send foreground bond to back using the **Change Position** ⟨icon⟩ 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 numbering, use the **Manual Numbering** ⟨icon⟩ or **Atom Chemical Properties** ⟨icon⟩ 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 allows you to remove 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 numbering, use the **Auto Renumbering** command (refer to
>
> Section 3.6.14), or the **Manual Numbering** ![#] and **Atom Chemical Properties**
>
> ![IAQ] 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 allows you to generate name(s) for the drawn structure(s). Note that this command is available both in the Structure and Draw modes. To obtain a name for one structure, select it, and then choose this command. The generated name will be inserted under the structure as a text string. To generate name for a mixture, select the required structures and choose this command. The generated name for the mixture will appear under the lower structure as a text string in one line.

> **Note** If only one structure is drawn or if you want to generate name for all the structures drawn in the workspace, you do not have to select structures.

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/name_lab/name/**.

Shortcuts:

    Keyboard: CTRL+SHIFT+I

    General toolbar: ![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 will appear:
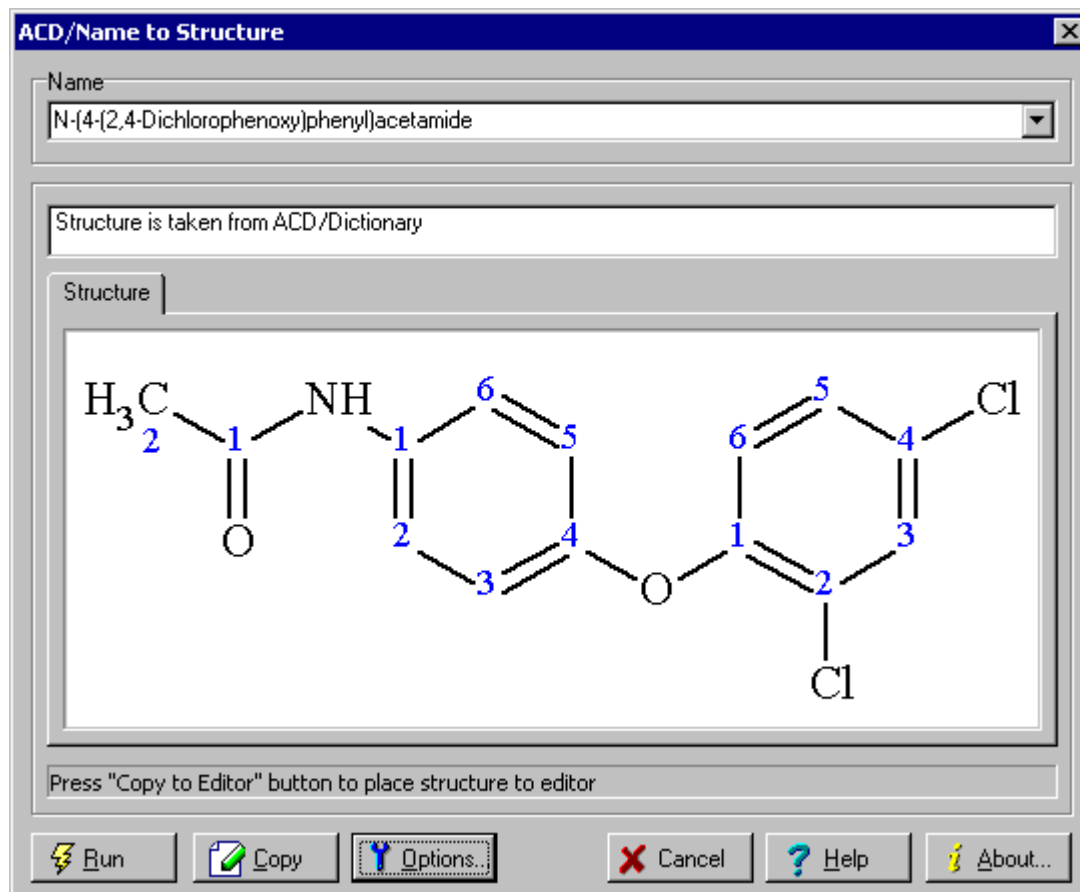
This dialog box contains the following options:

Option	Description
Name	In this box, specify the name and click **Run** to start the structure generation. Note that the drop-down list includes the names for which the structure generation process has been run before.
Warning(s)	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.
Structure	Displays the generated structure. If the system generates several structures for one name (e.g., pentanedithioic acid), the structures are placed into separate tabs. To view the structure, click the corresponding tab.

Option	Description
⚡ Run	Starts the structure generation process for the name specified in the **Name** box.
📝 Copy	Places the generated structure into the ChemSketch window.
Ŷ 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).
i About...	Displays the information about the current version of the program and the company-producer.

Shortcuts:

Keyboard: CTRL+SHIFT+G

General toolbar: 🗟

3.12.17.1 ACD/Name to Structure Options Dialog Box

The **ACD/Name to Structure Options** dialog box allows you to specify the structure generation options. To display it, in the **ACD/Name to Structure** dialog box, click **Options** Ŷ Options....

This dialog box contains the following options:

Option	Description
Numbering	If the **Show Numbering in Dialog** check box is selected, the atoms numbering will be displayed in the **ACD/Name to Structure** dialog box.
	If the **Copy to Editor with Numberin**g check box is selected, the atoms numbering will be displayed on the structure in case it is placed to the ChemSketch page.
	Note that if the generated structure is taken from ACD/Dictionary, numbering will not be displayed regardless of the options selected.
Warnings	If the **Ignore Warnings** option is selected, the program will generate structure(s) without displaying any warnings.
	If the **Report Warnings** option is selected, the generated structure(s) will be displayed together with warnings on its (their) reliability.
	Select the **Stop on Warnings** option, to stop the structure generation process if any problems appear. As a result, the corresponding warnings and no structure will be displayed.
	If the structure is found in ACD/Dictionary, it is displayed along with the corresponding warning.
Mark Undefined Double Bond Stereo	If this check box is selected, the program will generate structures with undefined double stereo bonds for names that do not contain the information on the double bond configuration.
Search ACD/Dictionary	If this check box is selected the system will search through ACD/Dictionary for the specified name in case the structure generation.
Check for SMILES Notation	If this check box is selected, the program will check if the entered name corresponds to the SMILES notation. If it does, the structure will be generated.
Check for InChI Notation	If this check box is selected, the program will check if the entered name corresponds to the InChI notation. If it does, the structure will be generated.

3.12.18 Generate > Stereo Descriptors

This command allows you to generate stereo descriptors for double bonds, chiral, and pseudo chiral centers. This command is available both in the Structure and Draw modes.

To generate stereo descriptors, select a structure or a set of structures and choose this command. Stereo descriptors appear on the selected structure(s) near the corresponding chiral center or double bond.

> **Note**   If no structure(s) is(are) selected in the workspace, stereo descriptors are automatically generated for all structures on the current page which have stereo centers or double bonds for which Z/E or R/S isomerism is possible.

S and **R** describe a chiral center configuration.

E and **Z** describe a double-bound configuration.

Small **r** and **s** describe configurations of pseudo chiral centers.

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 the color of stereo descriptors, from the **Options** menu, choose **Preferences**. In the dialog box that appears, click the **Structure** tab, and then select the appropriate color in the **Auto/Manual Numbering** box.

To generate special stereo descriptors for potential centers, and stereo warnings on the incorrectly defined stereoconfiguration, select a structure or a set of structures, specify options in the **Stereo Descriptors Options** dialog box, and choose this command.

After generation, the potential chiral centers will be marked with the asterix sign (*), atoms with the incorrectly defined stereoconfiguration will be marked with the question mark (?).

3.12.19 Generate Stereo Descriptors Options

This command displays the **Stereo Options** dialog box, which allows you to specify options for generating special warnings descriptors about missed or ambiguous definitions of stereoconfiguration. This option allows you to control the quality of chemical structure diagrams and avoid mistakes in structure representation and data calculations.

The dialog box contains the following options:

Option	Description
Take into Account Stereo Wedges Direction	If this check box is selected, the "up" and "down" wedges which specify stereo centers will be analyzed with regard to their directions (depending to which atom a narrow end is attached). If this check box is not selected, the sign ("up" or "down") of the stereo wedge doesn't depend on the direction. *If this check box is selected:* (**2R**)-2-chlorobutane (**2S**)-2-chlorobutane (**2R**)-2-chlorobutane *If this check box is not selected:* (**2R**)-2-chlorobutane (**2R**)-2-chlorobutane (**2R**)-2-chlorobutane -
Mark Undefined Chiral Centers	Select this check box to generate stereo descriptors for potential chiral centers. These centers will be marked with the asterisk sign (*).
Mark Incorrectly Defined Stereo	Select this check box to generate special warning descriptors to mark atoms with an incorrectly defined stereoconfiguration. They will be marked with a question mark (?).

3.12.20 Generate > SMILES Notation

This command generates SMILES (**S**implified **M**olecular **I**nput **L**ine **E**ntry **S**pecification) for the structure(s) displayed in the ChemSketch window. Note that this command is available both in the Structure and Draw modes.

If none of the displayed structures is selected, the SMILES's will appear for all the structures displayed. To generate SMILES for the definite structure, you should select it first.

2BStructure Mode

3.12.21 Generate > Structure from SMILES

This command generates structure(s) from SMILES (**S**implified **M**olecular **I**nput **L**ine **E**ntry **S**pecification). Note that this command is available both in the Structure and Draw modes.

Choosing this command displays the **Generate Structure from SMILES** dialog box where you can enter the required SMILES.

You can also generate structures from SMILES strings displayed in the ChemSketch window (either generated by using the **Generate > SMILES Notation** command, or placed in as a text manually). Just select the required SMILES string and choose this command. The generated structure will be placed below the SMILES string.

3.12.22 Generate > InChI for Structure

This command allows you to generate the InChI notation for a drawn structure.

The IUPAC International Chemical Identifier (InChI^{TM}) is a non-proprietary identifier enabling unambiguous identification of chemical substances for electronic and digital handling of chemical structural information.

An InChI label is generated by converting an input chemical structure (in the form of a 'connection table') to a unique and predictable set of ASCII characters. The InChI notation is a way of representing chemical compounds in a manner that does not depend on the way of drawing.

InChI procedures were developed under IUPAC project during the period 2000–2004. The technical development was carried out primarily at the US National Institute of Standards and Technology (NIST).

More information about InChI 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, which allows you to specify preferences for the InChI label generation.

This dialog box contains the following options:

Option	Description
InChI String	This option allows you to define whether or not 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—New to 11.0!	This option allows you to define whether or not to generate the auxiliary information for creating InChI string. It describes in a specific way the atom connections, numbers and coordinates.
	Note that AuxInfo can be different for the same structure, it depends on the structure drawing order.
InChI Key— New to 11.0!	This option allows you to define whether or not 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.
Mobile H Perception	This option allows you to define if the possible tautomerism should be taken into account or not. Clear this check box to include the information on the specific tautomer into the InChI notation.
Include Bonds to Metal	If this check box is selected, the InChI notation will include an information about bonds between metal and other atoms; otherwise, it will be ignored.
Stereo Options	This option allows you to choose whether to take into account stereoconfigurations in the drawn structure or not and how to treat them. You can choose between **Ignore**, **Absolute**, **Relative** and **Racemic** options that will be indicated in the corresponding section of the generated InChI notation.

Option	Description
Narrow End of Wedge Points to Stereocenter	This option defines how to treat stereo bond connecting two stereocenters. If the check box is cleared, the procedure treats such stereo bond as belonging to both stereocenters and having the same sense for both of them. If the check box is selected, only a narrow end will be taken into account and only one stereocenter will be defined in the generated InChI notation.

To generate InChI with the options specified in this dialog box, on the General toolbar, click **InChI for Structure** .

More information about InChI is available on the IUPAC website at www.iupac.org/inchi.

3.12.24 Generate > Structure from InChI

This command allows you to generate the structure for an InChI (IUPAC International Chemical Identifier) notation. You can use this option in both Structure and Draw modes:

- In the Structure mode; choose this command, and then in the **Generate Structure from InChI** dialog box that appears, type the InChI notation and click **OK**. An outline view of the generated structure is attached to your cursor, simply click to place it on the workspace. Note that you can flip the structure shadow by pressing TAB.

- In the Draw mode; type the InChI notation into the text box, and then choose this command. The generated structure appears on the ChemSketch page.

More information about InChI is available on the IUPAC website at www.iupac.org/inchi.

3.12.25 Search for Structure—Commercial version only!

This command starts the ACD/Search for Structure module that allows you to search for drawn chemical structure(s) in a variety of files without opening them. The following formats are supported:

- ACD/ChemSketch Document (.SK2)
- MDL molfile (.MOL)
- MDL SDfile (.SDF)
- ISIS/Sketch BIN-file (.SKC)
- CambridgeSoft ChemDraw CHM-file (.CHM)
- CambridgeSoft ChemDraw CDX-file (.CDX)
- Adobe Acrobat (.PDF) (created with ACD/Labs software)
- REACCS rxnfile (.RXN)
- Microsoft Word Document (.DOC)
- Microsoft Excel Document (.XLS)
- Microsoft PowerPoint Document (.PPT)
- ACD/Spec Database (.NDB; .ND5; .ND8)
- ACD/ChemFolder Database (.CFD)
- ACD/CNMR User Database (.CUD)
- ACD/HNMR User Database (.HUD)
- ACD/XNMR Database (.XDB)
- ACD/PhysChem User Database (.PCD; .LUD; .LU8; .PUD; .SUD)
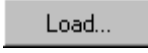
- ACD/ChromGenius Database (.CGB)
- ACD/NMR Predictor Internal Database (*NMR?.INT)
- ACD/Log*P* Internal Database (LOGP.INT)
- ACD/pK$_a$ Internal Database (PKA.INT)
- ACD/Solubility DB Internal Database (SOL?.INT)

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

Draw the fragment or structure you want to find and choose this command or click the corresponding button [icon] on the General toolbar. In the ACD/Search for Structure window that appears, you can specify the searching preferences and define the folders to be searched through.

This dialog box contains the following options:

Option	Description
Search Pattern	Displays the structure(s) to search for in the files specified in the **Look In** area.
Look In	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.
`*.MOL|*.SDF` [...]	In this box, you can specify the mask for the files to be searched through. You can either type it manually or click the 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.
Preview	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 📂 to display the shown structure either in ACD/ChemSketch or in the application specified in the **Search Options** dialog box (**Open** tab).
Search Results	This area displays the list of files where the query structure has been found. You can double-click any file from the list to open it either in ACD/ChemSketch or in any other selected application (depending on the option selected in the **Search Options** dialog box, **Open** tab).
Search	Starts searching. As you initiate the search, the Search button is transformed into the **Stop** button Stop that allows you to interrupt the search process and display the search results obtained so far.
Options...	Displays the **Search Options** dialog box where you can specify search conditions (for more information, refer to Sections 3.12.25.2–3.12.25.3).
Load...	Displays the **Load Search Results** dialog box where you can specify the name and location of a previously saved .SSF file containing search settings.
Save...	Displays the **Save Search** dialog box where you can specify the name and location of an .SSF file (Search for Structure Files format). The saved file will include the structure(s) to be searched, the folder and the file mask settings, as well as the search results (if any).
Status bar	**Files Processed**—indicates the number of files searched through so far. **Entries Found**—indicates the number of structures found so far. **Structures Compared**—reflects the number of structures compared to the search pattern so far. Reflects the current search location while searching or state on completion of the corresponding action: *Search Complete*, *Search Restored*, or *Search Saved*.
✗ Close	Closes the current window. Before the ACD/Search for Structure window is closed, the program prompts you to save the changes to the search settings.
i About	Displays information about your copy of ACD/Search for Structure, including the version number, the copyright, and your user registration information.

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: 🔲
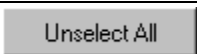
3.12.25.1 Look Through Files Dialog Box

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 this dialog box, in the **Look In** box of the ACD/Search for Structure window, click **Browse** [....].

This dialog box contains the following options:

Option	Description
List of Formats	Displays the formats (with the specified mask in broken brackets) supported by the ACD/Search for Structure module. To add the formats to the list of files to be searched through, select the corresponding check boxes. To set the mask for a specific format, highlight the format in the list and click **Change Mask**.
Change Mask...	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 format highlighted in the list to certain files by typing their mask(s) (for example, but* to search only the files whose names start with "but"). You can specify several masks separating them by a comma. Note that you should not type extensions because you can change the mask for the highlighted format only.
Clear Mask	Clears the mask(s) set for searching through the files of the format highlighted in the list. In this case, all files of the corresponding format will be searched.
Select All	Selects all of the file formats 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.
Unselect All	Clears all of the check boxes.

> **Note** For PDF format, you can search through the files created by means of ACD/ChemSketch only–all other files are ignored.

3.12.25.2 Search Options Dialog Box: General Tab—
Commercial version only!

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

To display this dialog box, in the ACD/Search for Structure window, click **Options** ` Options... ` (for more information, refer to Section 3.12.25).
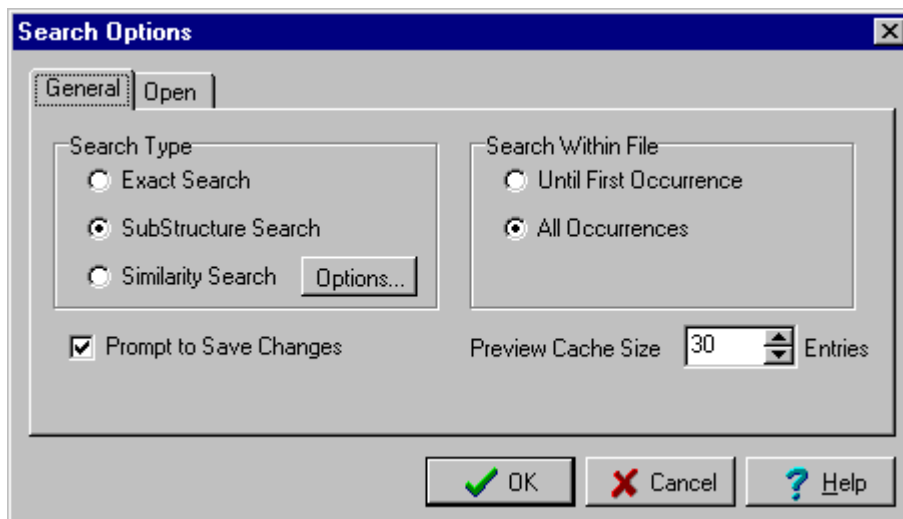
The **General** tab contains the following options:

Option	Description
Exact Search	If this option is selected, the specified files will be searched through for the presence of the search pattern as a standalone structure.
Substructure Search	If this option is selected, the program treats the currently displayed structure(s) as (a) substructure(s) and finds all structures containing the structure(s) as their structural fragment(s). Note that you can use the **Query Atom** and **Query Bond** tools to define the structure to be found (for more information, refer to Section 3.7.1–3.7.2).
Similarity Search	If this option is selected, the specified files will be searched through for the structure similar to that displayed in the **Search Pattern** box of the ACD/Search for Structure window. The options for the structures similarity can be specified by clicking **Options**; you can choose among the following similarity coefficients: **Tanimoto** **Dice** **Cosine** **Based on Hamming Distance** **Based on Euclidean Distance**
	For more information on these coefficients, refer to Section 3.12.25.4.

Option	Description
Prompt to Save Changes	If this check box is selected, each time you close the ACD/Search for Structure window, the program prompts you to save the results of search to an .SSF file if you have not done so.
Search Within File	If you select the **Until First Occurrence** 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. If the **All Occurrences** 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.
Preview Cache Size	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. In this box, you can specify the number of pages to be stored in cache.

3.12.25.3 Search Options Dialog Box: Open Tab— Commercial version only!

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

To display this dialog box, in the ACD/Search for Structure window, click **Options**   Options... (for more information, refer to Section 3.12.25).
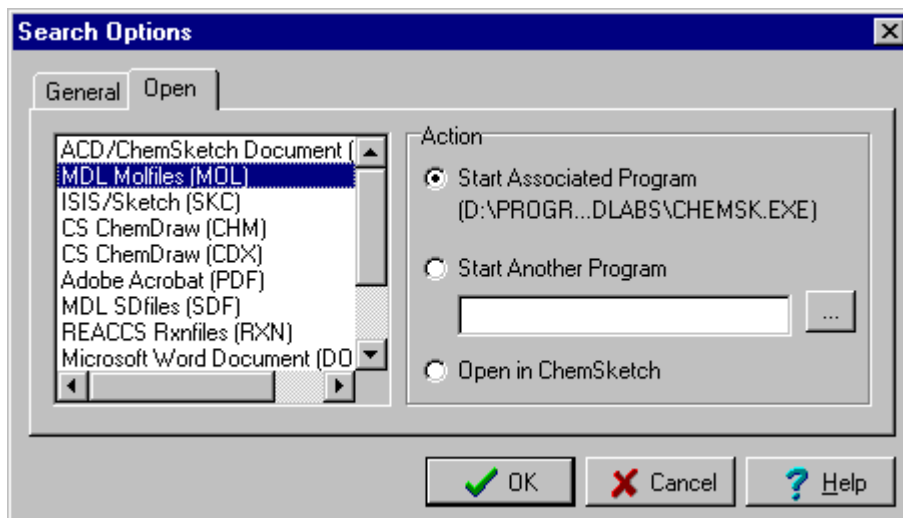
The **Open** tab contains the following options:

Option	Description
List of Formats	Displays the file formats that are currently supported by ACD/ChemSketch. When you click one of the formats in the list, the **Action** area is changed accordingly to show which program will open the found files.

2BStructure Mode

Option	Description
Action	In this area, specify which program should be used to open files of the selected format:
	If the **Start Associated Program** option is selected, the files of the selected format will be opened in the program currently associated with that format in the Windows system.
	If the **Start Another Program** 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).
	If the **Open in ChemSketch** option is selected, the found structure will be placed into the workspace of the ChemSketch window.

3.12.25.4 Similarity Search Options Dialog Box—Commercial version only!

This dialog box allows you to specify settings for searching structures according to a structure similar to a target one (that is currently displayed in the ChemSketch window).

This dialog box appears when you click **Options** ![Options...] in the **Search Options** dialog box.

This dialog box contains the following options:

Option	Description
Select Similarity Coefficient	Displays the list of similarity coefficients that can be applied during the similarity search. To apply the desired coefficient, select its check box.
Show with Coefficient >=	In this box, specify the similarity coefficient that will serve as a filter for the found structures. During the similarity search, the program generates a similarity coefficient 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.

3.12.26 Calculate > "*Property Name*" / All Properties

This set of commands allows you to calculate one or all of the properties for the currently selected structure or fragment. The following properties are available:

- Molecular formula
- Formula weight
- Composition
- Molar refractivity
- Molar volume

- Parachor
- Index of refraction
- Surface tension
- Density
- Dielectric constant
- Polarizability
- Monoisotopic, nominal and average mass

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

As you choose one of the commands, the corresponding property is calculated for the structure and the **Calculation Results** dialog box appears displaying the data. To copy the results to the ChemSketch window near the structure, click **Copy to Editor**.

> **Note** If there are several structures drawn in the workspace and none is selected, the properties are calculated for all of these structures (treating them as one composite structure), if possible. If it is impossible to calculate a property, it is labeled as "Not available".

If you choose the **All Properties** command, the results are represented as a set of rows. You can select the properties to be placed by the structure: holding down CTRL, click the desired properties to select them, and then click **Copy to Editor**. Clicking **Cancel** will close the dialog box without copying the results to the workspace.

> **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 > Select Properties to Calculate

This command allows you to define the properties to be calculated when you choose the **Calculate > Selected Properties** command from the **Tools** menu.

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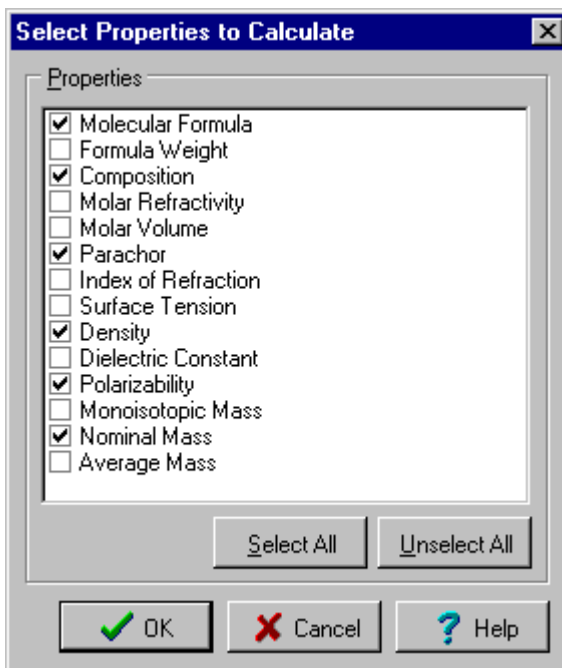
This dialog box contains the following options:

Option	Description
Properties	Lists the available properties. To define the properties to be calculated, select the check boxes adjacent to the required properties.
Select All	Selects all of the properties in the list.
Unselect All	Clears the check boxes of all the properties in the list.

3.12.28 Calculate > Selected Properties

This command calculates the properties selected in the **Select Properties to Calculate** dialog box (for more information, refer to the previous sections).

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 shows the contents of available templates, either standard (built-in) or custom (user-defined).

This dialog box contains the following options:

Option	Description
Structure Draw	Allows you to choose either the Draw or Structure mode. This mode will be active when you place the selected template on the ChemSketch page.
Sugars: beta-D-Pyr	This box contains templates listed in the **Template Organizer** (for more information, refer to Section 3.13.2). To load a template, select it from the list.
1(4) Haworth Formulae	In this box, you can choose the desired page of a multi-page template.
◄☐ ☐►	Allow you to move from page to page within the multi-page template.
Organizer	Displays the **User Template Window Organizer** dialog box where you can manage templates (for more information, refer to Section 3.13.2).
Template Tabs	The upper part displays the list of "fixed" templates, i.e., templates whose names are displayed in the Template Window dialog box every time you open it. You can specify your own "fixed" templates using the **User Template Window Organizer** dialog box (for more information, refer to Section 3.13.2).
The lower part displays the list of templates that have been recently chosen from the list of available templates at the top of the window. If you use some templates frequently and want them to be present in the **Template Window** dialog box every time you open it, you can place them into the "fixed" list above by selecting the template names in the **User Template Window Organizer** dialog box.
Preview	Displays the contents of the template currently selected in the list.

To insert a template:

1. Click **Structure** [Structure] or **Draw** [Draw] in the **Template Window** dialog box to indicate which mode is to be active when you place the selected template on the ChemSketch page.

2. From the left row of tabs or from the drop-down list at the top, choose a template. The contents of the template appear. If there is more than one page in a template, you can switch from page to page using [◄⬚] and [⬚►].

3. Click a template item. The program switches to the ChemSketch window in the **Structure** or **Draw** mode (depending on which button you have selected) with a template attached to the cursor. Note that an outline view of the template item is attached to your cursor.

> **Note**   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 suitable 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. (Note that if the item is a structure or fragment, it attempts to attach itself to the appropriate location as you move it over the workspace; simply click to place it at the insertion point.) Every time you click, you place another copy of the item on the workspace.

5. To cancel, choose any button on the toolbar or right-click in the workspace.

> **Note**   You can flip the template shadow by pressing TAB.
>
> When inserting template of a chemical structure, if you click an atom of the drawn structure holding down SHIFT, the atom of the template will replace the atom you click (template will be attached without a bond).

Shortcuts:

Keyboard: F5

General toolbar:
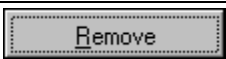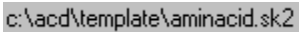
3.13.2 Template Organizer

This command displays the **User Template Window Organizer** dialog box, which allows you to manage the standard (built-in) and custom (user-defined) templates. Using this dialog box you can create a template, change the name of the file associated with a template, and remove, rename, and modify the template's contents.
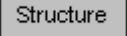

This dialog box contains the following options:

Option	Description
Templates	Displays the list of the available templates. To see the list of all the templates (both standard and user's), select the **All** option. The templates with selected check boxes are included into the list of "fixed" templates in the **Template Window** dialog box, i.e., templates whose names are displayed in this dialog box every time you switch to it. Note that only ten templates can be placed as "fixed" at a time. To include the template into the **Template Window** dialog box, click any tick and then click the box corresponding to the required template.
Standard / User / All	Options of this box allow you to switch between the lists of **Standard** (built-in), **User** (added by the user), and **All** templates.
Fixed / Available	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 to the **Template Window** dialog box at a time.
New...	Displays the **Create User Template** dialog box where you can choose a file to be saved as a user template and specify the template name. As you click **OK**, the template will be added to the **Template** box.

Option	Description
Modify...	Choose the template from the list and click this button to display the **Modify Template** dialog box. In this dialog box, you can edit the template name and a file serving as a template.
Remove	Removes the highlighted template from the list. Note that this removes only the reference to the corresponding .SK2 file, but not the file itself.
Open Document	This button loads an .SK2 file associated with the highlighted template into the ChemSketch page for editing.
c:\acd\template\aminacid.sk2	Displays the location of a document associated with the template highlighted in the list.

Note that the only difference between the template file and a usual file 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 usual 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 document by previewing its contents in the preview field of the **Template Window**.

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. As soon as you save your document, the **Save User Template** dialog box appears where you should specify the name for your template to be associated with your document.

As soon as the document is saved as a template, its contents becomes available in the **Template Window** dialog box as an additional tab and in the **Template Organizer** dialog box in the list of user templates (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 containing the most frequently needed radicals for a quick structure drawing.
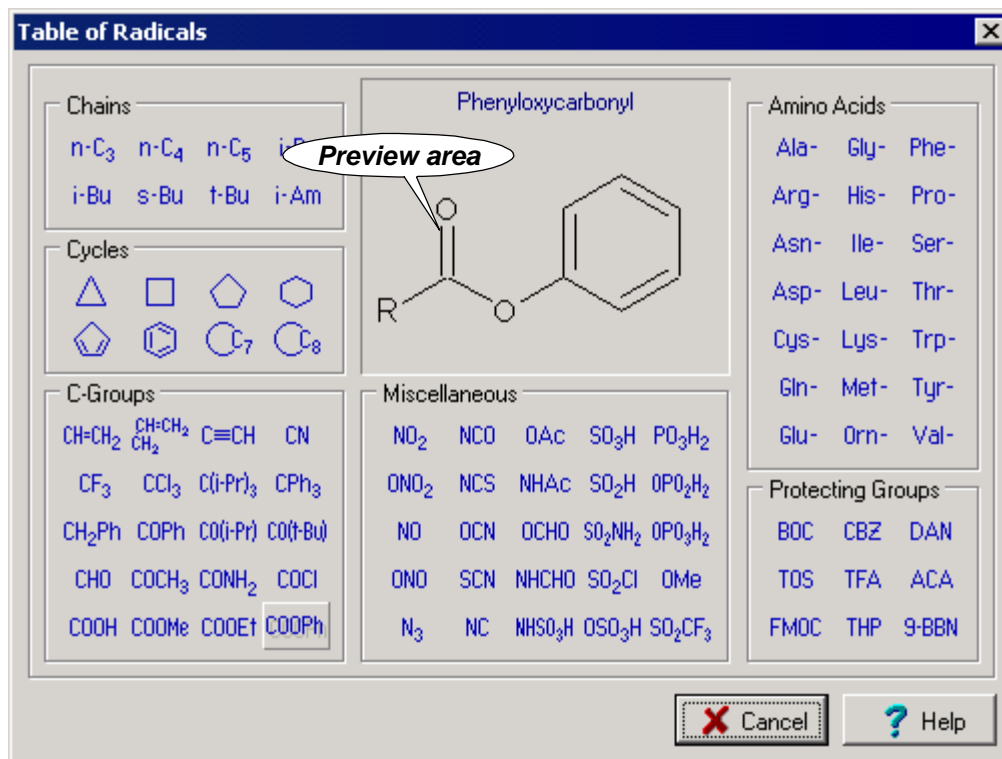
When you point to a radical, information about it appears in the Preview area. Note that the "R" in the radical structure denotes the position of attachment to other structures in the drawing area.

To choose a radical for drawing, click the required radical button. The Table of Radicals will be closed and a shadow will be attached to the cursor. Click in the empty space to insert a non-bonded structure of the chosen radical or click any atom to link it up to the chosen radical. To replace any atom of the drawn structure with the atom of the radical (i.e., the radical will be attached without a bond), click the corresponding atom holding down SHIFT when inserting the radical structure.

You can flip the radical shadow by pressing TAB. You can use the radical shadow as many times as you want until you click with the right mouse button to cancel this mode.

When a radical is chosen from the Table of Radicals, its corresponding button is automatically added to the References toolbar (for more information, refer to Section 3.8). To remove the radicals from the References toolbar, double-click an empty space on the toolbar.

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	
Action	*pulled position* ( )	*pushed position* ( )
To highlight an element and display the photo and detailed information about it	point to the desired element	click the desired element
To be able to insert the selected element into the workspace	click the desired element	click **OK**

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:

3.13.6 Dictionary—Commercial version only!

This command displays the **ACD/Dictionary** dialog box.
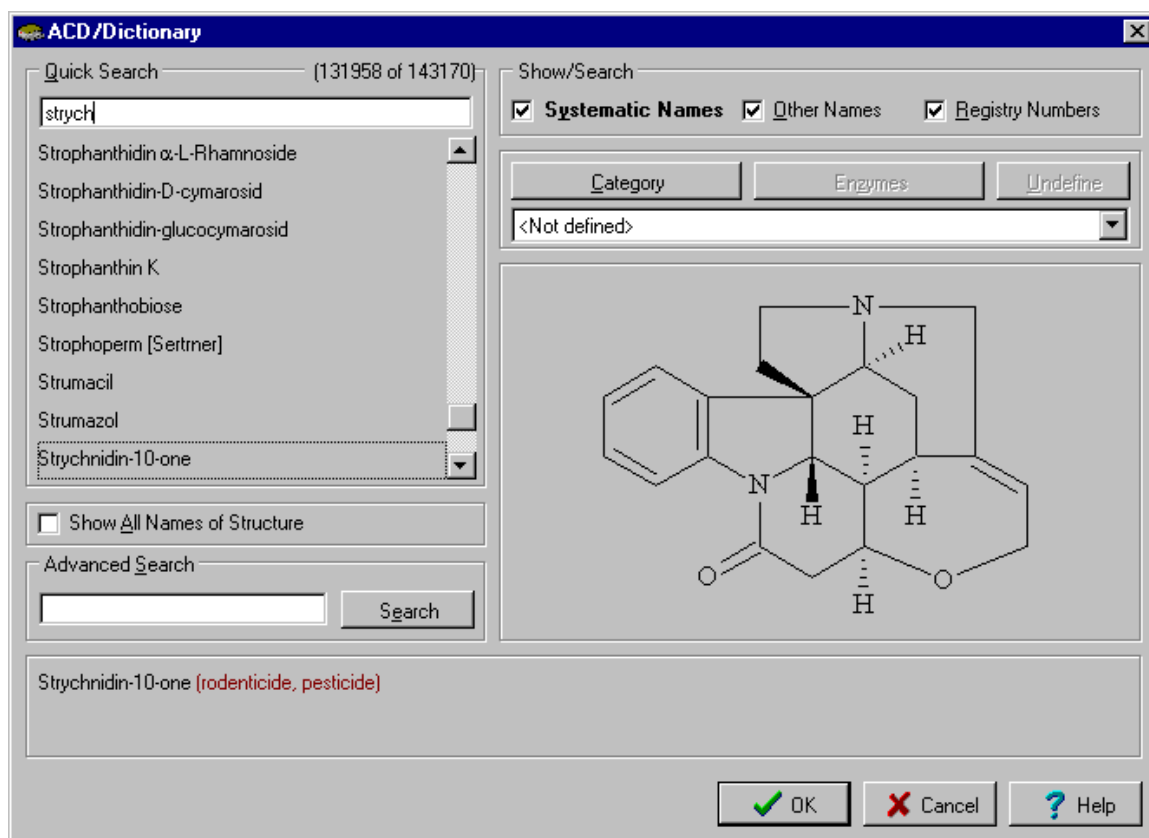
ACD/Dictionary is a program from ACD/Labs which allows you to find chemical structures according to their systematic or non-systematic names (as well as according to the parts of name), therapeutic category or inhibited enzymes, and registry numbers. You can copy these structures to other ACD/Labs programs and to Windows applications.

If there is structure(s) drawn or selected in the workspace and the **Auto Search Structure** option is marked with a tick, 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: ⬗

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:

This tab contains the following options:

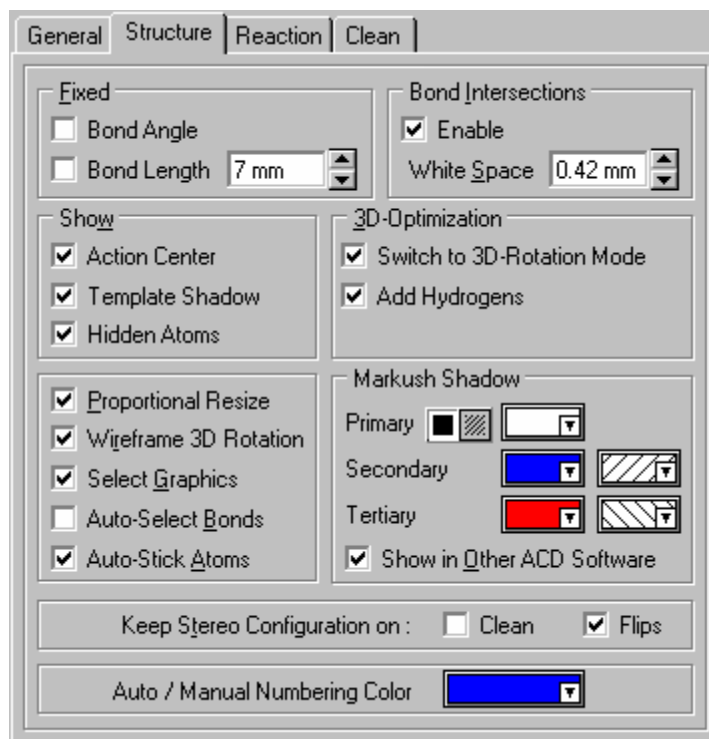| Option	Description
View	In this area, you can specify the objects to be displayed: The **Ruler** check box switches on/off the display of the ruler. The rulers are useful for determining the size and position of objects. The **RSS** check box switches on/off the display of the RSS News bar. For more information on the RSS options, refer to Section 2.5.1. The **Guides** check box switches on/off the display of the guides that appears on each ruler indicating the position of the cursor. Note that this option is available if the Ruler check box is selected. The **Palette** check box switches on/off the display of the Color palette (refer to Section 2.4). In the **Measurement Units** box, specify the units to be used for measurements in all dialog boxes.
Borders	Select the **Printable Area** 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 **Page Margins** check box to display the dotted lines showing the margins of the page. You can set the margins in the **Page Setup** dialog box (**File** menu).
Highlight Color	In this box, you can specify the color to be used for highlighting when you point to structure elements and drawing objects.
Grid	Allows you to specify the way the grid should be arranged: in the form of rectangles vertically hexagonally horizontally hexagonally
Visible	This check box controls whether to show or hide the grid. This is also controlled by the **Show Grid** command (**Options** menu).
Snap on Grid	If this check box is selected, objects "stick to" (become automatically aligned with) the grid (either visible or not) when you move or create them. This is also controlled by the **Snap On Grid** command (**Options** menu). Note that if this option is enabled, the **Fixed Bond Length** and **Bond Angle** features (**Structure** tab) are ignored.
Horizontal Step / Vertical Step	In the **Horizontal Step** box, you can specify the horizontal distance* between the grid points of the rectangular or horizontally hexagonal grid. In the **Vertical Step** box, you can specify the vertical distance between points for rectangular or vertically hexagonal grid.*
Keep Draw Tool Active	If this check box is selected, any of the drawing tools from the Drawing toolbar (except the **Text** tool ▦) remains enabled until you click or right-click in the workspace. If this check box is cleared, the **Select/Move/Resize** tool ↳ becomes active every time after you have used a tool.
Informative Cursor	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.
Use Antialiasing— New to 11.0!	Select this check box to automatically remove the aliasing of drawn lines and curves.
Directories	In this area, you can specify the name of folders where some configuration information will be stored. In the **Private** box, you can specify the folder for recording the configuration of ChemSketch program (TEMPLATE.CFG and QRSTYLES.STL files). In the **Default** box, you can specify the folder which you want to become current for the first time when you open the **Save As**, **Open**, **Import**, or **Export** dialog boxes in the current work session.

3.14.1.2 Preferences Dialog Box: Structure Tab
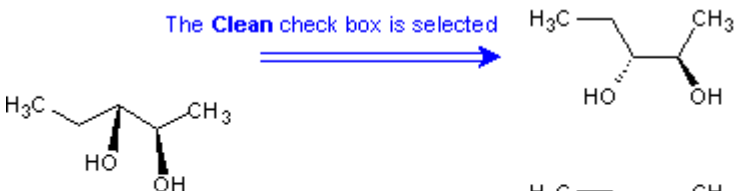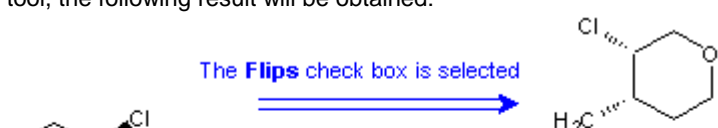
On the **Structure** tab, you can define the preferences for the structures' display and drawing.

This tab contains the following options:

Option	Description
Fixed	In the **Fixed** area, you can control the structure drawing.
	If the **Bond Angle** check box is selected, you will be able to draw bonds at an angle multiple to 15°.
	If the **Bond Length** 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 **Snap on Grid** check box is selected on the **General** tab of this dialog box. To make the check boxes in the **Fixed** area available, clear the **Snap on Grid** check box.
Action Center	Select this check box to view the special sign showing the center of rotation or resizing when you use the **Select/Rotate/Resize** [icon] tool. This will help you see the point relative to which the objects are resized or rotated.
Template Shadow	If this check box is selected, the shadow of the template structure will be displayed near the cursor when you use the **Instant Template** tool or use templates from the **Table of Radicals** or **Template Window**.
Hidden Atoms	If this check box is selected, the hidden atoms will be displayed when you point to them on the structure.
Proportional Resize	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.

Option	Description
Wireframe 3D Rotation	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.
Select Graphics	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 pluses and arrows. If this check box is cleared, you can only manipulate structures in the Structure mode.
Auto-Select Bonds	If this check box is selected, as you hold down SHIFT and click two atoms or bonds with the **Select/Move** 🔍 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.
Auto-Stick Atoms	Select this check box if you want atoms or bonds to be automatically stuck either in the Move or Template modes (refer to Sections 3.6.1and 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*.
Bond Intersections	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.
3D-Optimization	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.
Markush Shadow	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.

Option	Description
Keep Stereo Configuration on	In this area, select the **Clean** check box to keep the configuration of stereo centers unchanged when applying the **Clean Structure** command. For example: Select the **Flips** check box to keep the configuration of stereo centers unchanged when using the **Flip on Bond**, **Flip Top to Bottom**, or **Flip Left to Right** tools. For example, when you apply the **Flip Left to Right** tool, the following result will be obtained:
Auto/Manual Numbering Color	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.

3.14.1.3 Preferences Dialog Box: Reaction Tab

On the **Reaction** tab, you can customize the appearance of reaction elements.
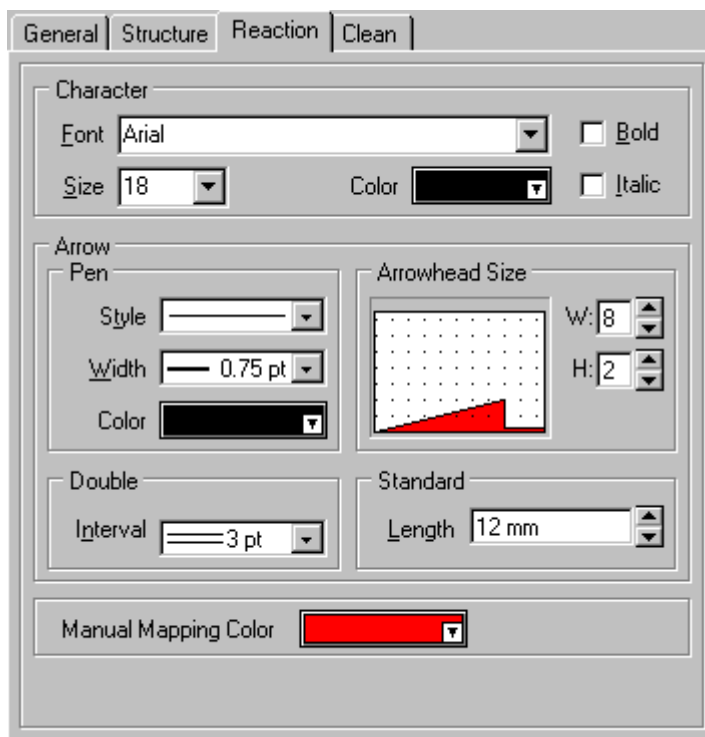
This tab contains the following options:

Option	Description
Character	In this area, you can specify the text style for reaction pluses (for more information, refer to Section 3.6.14).
Pen	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.
Arrowhead Size	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.
Double	In this area, you can specify the space between the lines of a double reaction arrow. Choose the required sample in the **Interval** box.
Standard	In this area, you can set the default length of a reaction arrow. Type the required value in the **Length** box.
Manual Mapping Color	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).

3.14.1.4 Preferences Dialog Box: Clean Tab
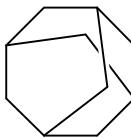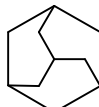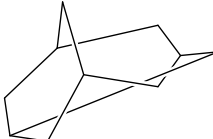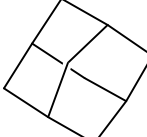
On the **Clean** tab, you can specify what method to use when applying the **Clean Structure** command.
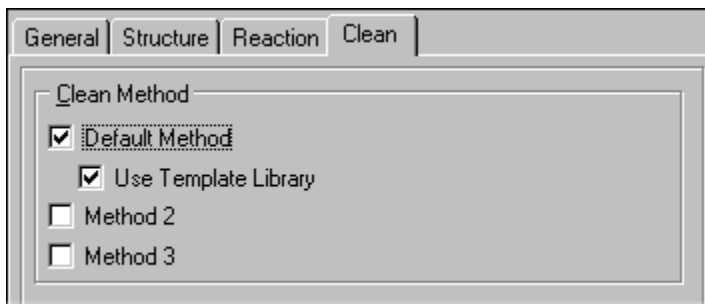
You can choose the required method of structure representation by selecting the corresponding check boxes. If you select several check boxes, all of them will be applied one after another every time you click **Clean Structure** on the Structure toolbar, or choose the **Clean Structure** command from 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:

Clean Method	Structure Representation
Default Method without Template Library	
Default Method with Template Library	
Method 2	
Method 3	

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 objects or creating new ones. Note that the grid can be enabled even if the grid lines are hidden.

> **Note**   To change the grid density and type, use the **Preferences** dialog box options.

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:

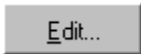| Option	Description
List of add-ons	This box lists supplementary applications that can be used to enhance the program's possibilities. To edit the list, use the buttons to the right. Select the check boxes of those add-ons that are to be added to the **Add-Ons** menu and/or Top toolbar (if this is specified 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.
Add...	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.
Edit...	Displays the dialog box where you can edit the properties of the add-on selected in the list.
Delete	Removes the add-on selected in the list.
Add-on location	This box displays the location of the add-on currently selected in the list.
Add-on description	In this box, view the description of the add-on selected in the list above.

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.

This dialog box contains the following options:

Option	Description
Installed Programs	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.
New...	This button allows you to install a ChemBasic program and add its name to the list. Clicking this button displays the **ChemBasic Program** dialog box where you can specify the program, its shortcut button, and hint. For more information, refer to Section 3.14.8.1.
Modify...	This button allows you to modify the name, shortcut, or location of the program currently highlighted in the list. Clicking this button displays the **ChemBasic Program** dialog box. For more information, refer to Section 3.14.8.1.
Delete	Deletes the currently highlighted program from the list and uninstalls the corresponding .BAS file.

3.14.8.1 ChemBasic Program Dialog Box

In this dialog box, you can define some options for running the selected ChemBasic program.

This dialog box appears when, in the **ChemBasic Organizer** dialog box, you click either the **Modify** or **New** button.

This dialog box contains the following options:

Option	Description
Name	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.
File	In the **File** area, specify the name and location of a ChemBasic program to be installed.
Toolbar	In the **Toolbar** area, specify the toolbar to which the shortcut button should be placed: • General toolbar (refer to Section 3.5); • Additional ChemBasic toolbar (that will appear between the General and Structure toolbars); or • Structure toolbar (refer to Section 3.6).
Bitmap File	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.

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 ACD/Labs Online (I-Lab)

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, H(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://www2.acdlabs.com** address;
    - ***I-Lab: Intranet Edition:*** Access to the server where I-Lab: Intranet Edition is installed.
- 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 keys 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 Close All

This command closes all of the programs from the ACD/Labs package that are currently running. To close only one program, from the **File** menu, choose **Exit**, or, on the title bar, click **Close** ✕.

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 can be downloaded for free 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.*
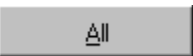
3.19.6 Message Box Preferences

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.
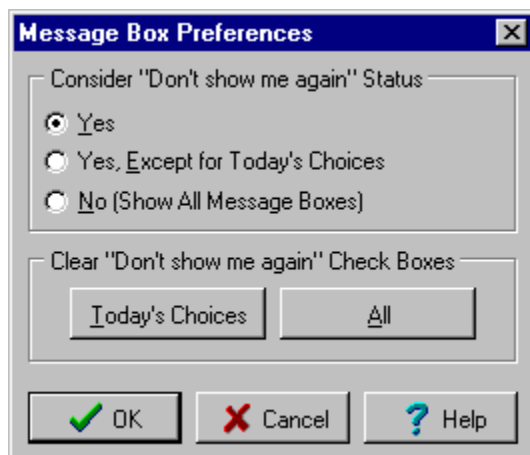
This dialog box contains the following options:

Option	Description
Consider "Don't show me again" Status	
Yes	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.

Option	Description
Yes, Except for Today's Choice	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.
No (Show All Message Boxes)	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.

	Clear "Don't show me again" Check Boxes
Today's Choices	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.
All	Clears the **Don't show me again** check boxes everywhere thus allowing you to display all the message boxes that can occur.

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 the 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 the 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/**.

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:

Option	Description
Go to the ACD/Labs Bug Report Page	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 (http://www.acdlabs.com/feedback/bugs.html) will be opened.
Send E-mail to ACD/Labs Bug Processing Center	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.

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 describes in detail the options, tools and features available in the Draw mode. You will be acquainted with the following:

- The general capabilities of the Draw mode;
- Draw mode interface at a glance, and
- Detailed description of each command, tool, and interface part available in the Draw mode.

To switch to the Draw mode, on the General toolbar, click **Draw** Draw .
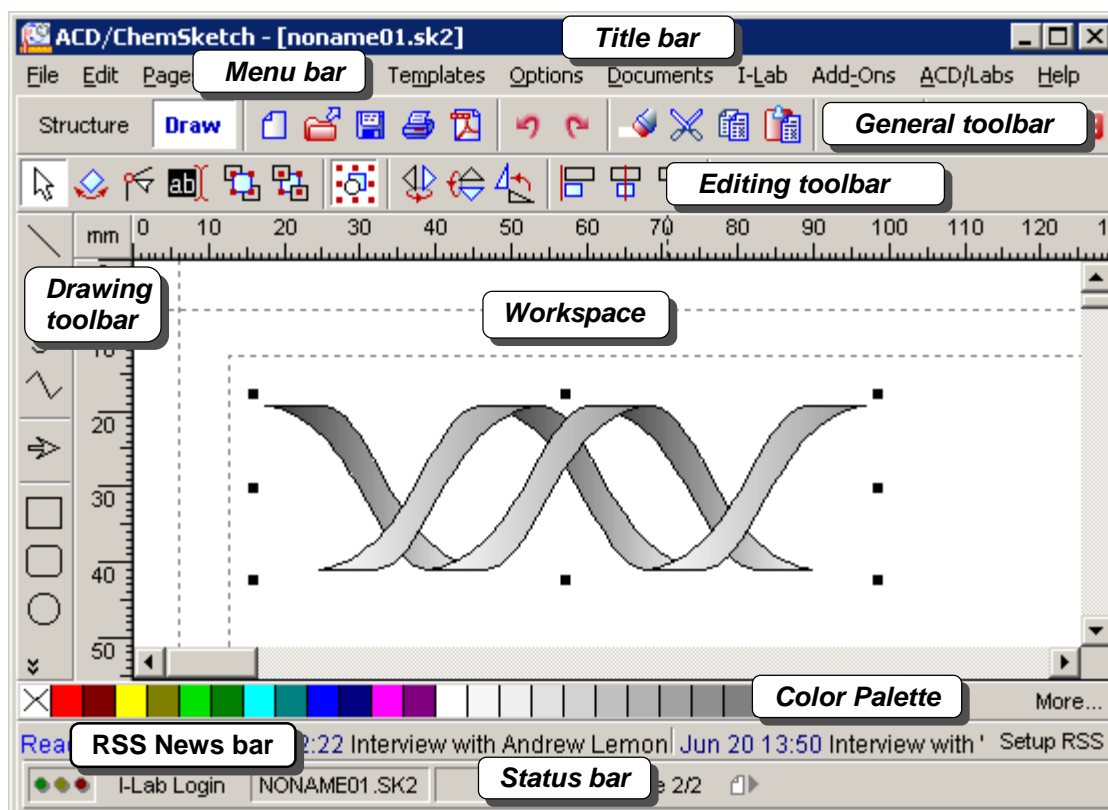
4.2 General Information

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 screen with the Draw mode enabled. The names and positions of the toolbars and the other elements, to be used throughout this manual, are introduced.

This table gives the short description of each interface element designated in the above picture:

Interface Element	Function
Title bar	This bar 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).
Menu bar	This bar contains a series of words. Each word links to a list ('menu') of related commands for working in the ChemSketch window in the Draw mode (for a detailed description of each menu and the commands it contains, refer to Sections 4.8–4.18).
General toolbar	This toolbar includes tools that are present in both Structure and Draw modes and will help you with tasks relevant to both modes such as: saving, opening 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).
ChemBasic toolbar	This toolbar includes additional tools that extend the functionality of ACD/ChemSketch. Note that the ChemBasic toolbar is present in both Structure and Draw modes if you have the Goodies tools previously installed (for more information, refer to Appendix C).

Interface Element	Function
Editing toolbar	This toolbar is only present in the Draw mode. It contains tools 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). For more information, refer to Section 4.6.
Drawing toolbar	This toolbar contains buttons used for creating graphical objects such as lines, rectangles, text boxes, etc. (for more information, refer to Section 4.7).
Workspace	The workspace is the current ChemSketch page 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).
Status bar	This bar contains information that may be useful for the current moment: name of the opened .SK2 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.

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.
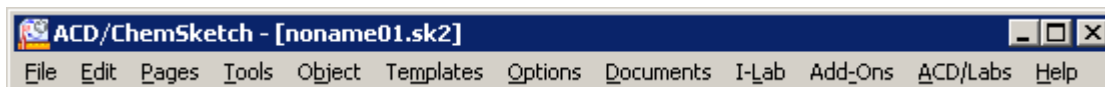
For detailed information on the commands that are available from the menus of the ChemSketch window in the Draw mode, refer to Sections 4.8–4.18.

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:

Button	Function
	Allows you to select, move, and resize objects (for more information, refer to Section 4.6.1).
	Allows you to select, move, and rotate objects (for more information, refer to Section 4.6.2).

Button	Function
	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.
	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.
	Brings the selected background objects to the foreground (for more information, refer to Section 4.12.2).
	Sends the selected foreground objects to the background (for more information, refer to Section 4.12.3).
	Groups/ungroups the selected objects and allows you to place data into tables (for more information, refer to Section 4.12.1).
	Turns the selected object(s) about the vertical axis (for more information, refer to Section 4.12.4).
	Turns the selected object(s) about the horizontal axis (for more information, refer to Section 4.12.5).
	Rotates the selected object(s) by 90° (for more information, refer to Section 4.12.6).
	Aligns the selected objects horizontally to the left (for more information, refer to Section 4.12.7).
	Aligns the selected objects horizontally to center (for more information, refer to Section 4.12.7).
	Aligns the selected objects horizontally to the right (for more information, refer to Section 4.12.7).
	Aligns the selected objects vertically to the bottom (for more information, refer to Section 4.12.8).
	Aligns the selected objects vertically to the center (for more information, refer to Section 4.12.8).
	Aligns the selected objects vertically to the top (for more information, refer to Section 4.12.8).

> **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

This button enables the **Select/Move/Resize** tool allowing you to select, move, and resize graphical objects created both 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 should do to select objects:

To Select	Do This
One object	Click the object or drag around the object.
Multiple objects	Hold down SHIFT when selecting as described in the previous action.
All the objects in the workspace	Press CTRL+A. Note that pressing CTRL+A again will deselect all of the objects.

The table below summarizes the actions you should do to move objects:

To Move	Do This
Selected object(s)	Point to the object so that the contour appears around it and drag.
Selected object(s) leaving its copy behind	Hold down CTRL while dragging.
Selected object constraining the object's movement	Hold down SHIFT while moving; in this case, the movement of the selected object is constrained to the X or Y axis.

> **Note** If the **Informative Cursor** check box in the **Preferences** dialog box (**General** tab) is selected, the new object's coordinates (relative to its original location) are displayed near the cursor.

The table below summarizes the actions you should do to resize objects:

To Resize	Do This
Selected object relative to its side or corner	Point to the selection handle so that the cursor changes to a two-way arrow (↕, ↔, ↘, or ↗), and drag.
	Dragging the top / bottom side selection handles resizes the object's height, dragging the left / right side handles—width; and dragging the corner handles resizes the object proportionally in all directions.
Selected object relative to its center	Hold down CTRL when dragging the selection handles as described above.
Selected object proportionally to 5% of its size	Hold down SHIFT when dragging the **side** selection handles as described above.
Selected object so that the height and width change independently	Hold down SHIFT when dragging the **corner** selection handles as described above.

> **Note** If the **Informative cursor** check box in the **Preferences** dialog box (**General** tab) is selected, the percentage of resizing will be displayed by the cursor.

You can quickly switch between this tool and the **Select/Move/Rotate** ⬦ tool by right-clicking in the workspace or by clicking any selection handle.

4.6.2 Select/Move/Rotate Button

This button ⬦ enables the **Select/Move/Rotate** tool allowing you to select, move, and rotate objects created both 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 table below summarizes the actions you should do to select objects:

To Select	Do This
One object	Click the object or drag around the object.
Multiple objects	Hold down SHIFT when selecting as described in the previous action.
All the objects in the workspace	Press CTRL+A. Note that pressing CTRL+A again will deselect all of the objects.

The table below summarizes the actions you should do to move objects:

To Move	Do This
Selected object(s)	Point to the object so that the contour appears around it and drag.
Selected object(s) leaving its copy behind	Hold down CTRL while dragging.
Selected object constraining the object's movement	Hold down SHIFT while moving; in this case, the movement of the selected object is constrained to the X- or Y-axis.

> **Note** If the **Informative Cursor** check box in the **Preferences** dialog box (**General** tab) is selected, the new object's coordinates (relative to its original location) are displayed near the cursor.

The table below summarizes the actions you should do to rotate objects:

To Rotate	Do This
Selected object around its center	Point to the selection handle so that the cursor changes to ⟲ and drag.
Selected object in 15 degree increments	Hold down SHIFT when rotating as described in the previous action.

> **Note** If the **Informative Cursor** check box in the **Preferences** dialog box (**General** tab) is selected, the angle of rotation will be displayed by the cursor.

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

This button ⟦⬀⟧ enables the **Edit Nodes** tool allowing you to 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:
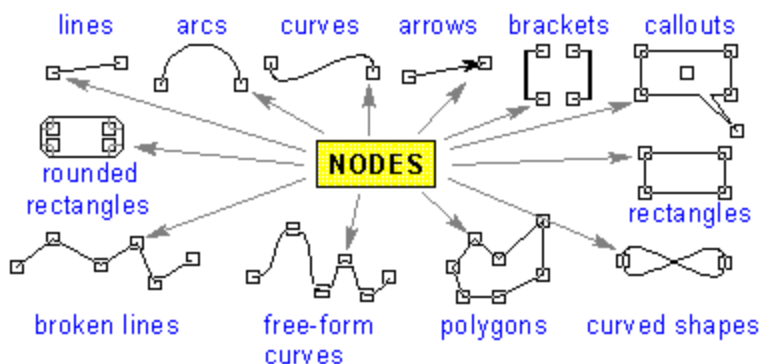
> **Note** Only one object can be selected at a time when the **Edit Nodes** tool is active.

The function of the **Edit Nodes** tool varies depending on the type of object selected:

Object Type	Function
Line/Arrow/Curve/Polygon/ Curved shape	Changing the shape by moving nodes and control points and using the Node toolbar.
Rectangle	Rounding corners by moving nodes.
Rounded Rectangle	Changing the radius of corners by moving nodes.
Arc	Changing the length by moving nodes.
Brackets/Callout	Modifying the size and shape by moving nodes.

Note **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.
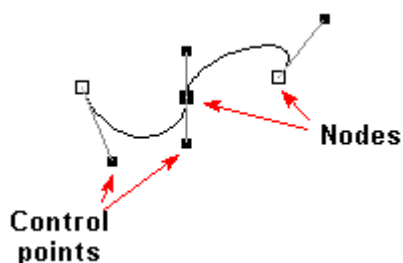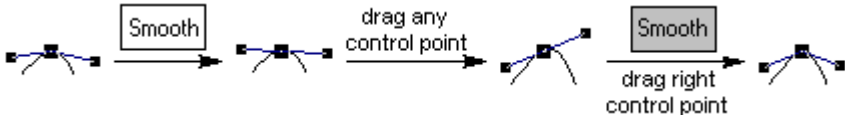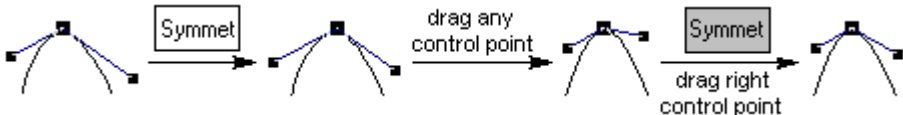
4.6.3.1 Node Toolbar

The Node toolbar appears when you click **Edit Nodes** 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).

Button	Function
Connect Vertices	Connects end nodes of a selected free-form curve or broken line with a straight line.
Disconnect Vertices	Erases the segment between the two selected adjacent nodes.
Add Node	Adds a node between the two selected adjacent nodes. Each additional click on this button will add new nodes between the existing ones.
Delete Nodes	Deletes the selected nodes.
Convert to Line	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.
Convert to Curve	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.

Button	Function
Smooth	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 **Smooth** button to disable this function.
Symmet	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 **Symmet** button to disable this function.
Align Left	Aligns the selected nodes horizontally to the left—relative to each other.
Center Horizontally	Aligns the selected nodes horizontally to the center—relative to each other.
Align Right	Aligns the selected nodes horizontally to the right—relative to each other.
Align Bottom	Aligns the selected nodes vertically to the bottom—relative to each other.
Center Vertically	Aligns the selected nodes vertically to the center—relative to each other.
Align Top	Aligns the selected nodes vertically to the top—relative to each other.

> **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

This button enables the **Edit Text** tool allowing you to 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** 🔲, **Text** 🔲, or **Artistic Text** T tool. The Text toolbar replaces the right part of the Editing toolbar. It contains the following buttons for formatting text:

Button / Box	Function
Arial ▾	In this box, you can specify the font style for the selected text or for the text to be typed.
12 ▾	In this box, you can specify the font size for the selected text or for the text to be typed.
B	Applies the bold formatting (e.g., **text**) to the selected text or to the text to be typed.
I	Applies the italic formatting (e.g., *text*) to the selected text or to the text to be typed.
U	Applies the underlined formatting (e.g., <u>text</u>) to the selected text or to the text to be typed.
Ө	Applies the strikethrough formatting (e.g., ~~text~~) to the selected text or to the text to be typed.
S+	Applies the superscript formatting (e.g., ^{text}) to the selected text or to the text to be typed.
S-	Applies the subscript formatting (e.g., $_{text}$) to the selected text or to the text to be typed.
Ω	Transforms characters of the selected text or the text to be typed to Greek symbols.
≣	Aligns the text to the left.
≣	Centers the text in the text box.
≣	Aligns the text to the right.
≣	Stretches the text so that it fills the whole lines between the left and right borders of a text box.
🔲	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.
🔲	Saves the current font and paragraph attributes as default.

> **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:

Button	Function
	Allows you to draw straight lines (for more information, refer to Section 4.7.1).
	Allows you to draw arcs (for more information, refer to Section 4.7.2).
	Allows you to draw curves of a predefined shape (for more information, refer to Section 4.7.3).
	Allows you to draw free-form curves and broken lines (for more information, refer to Section 4.7.4).
	Allows you to draw arrows of different shape (for more information, refer to Section 4.7.5).
	Allows you to draw rectangles (for more information, refer to Section 4.7.6).
	Allows you to draw rectangles with rounded corners (for more information, refer to Section 4.7.7).
	Allows you to draw ellipses and circles (for more information, refer to Section 4.7.8).
	Allows you to draw free-form shapes (for more information, refer to Section 4.7.9).
	Allows you to insert images (for more information, refer to Section 4.7.10).
	Allows you to insert text into the workspace (for more information, refer to Section 4.7.11).
	Allows you to draw table of specified size (for more information, refer to Section 4.7.12).
	Allows you to draw brackets of different types (for more information, refer to Section 4.7.13).
	Allows you to draw callouts (for more information, refer to Section 4.7.14).
	Allows you to create templates for ACD/SpecManager reports (for more information, refer to Section 4.7.15).

> **Note**   The toolbar can be customized according to your preferences; for more
>   information, refer to Section 2.2.1.

4.7.1 Line Button

This button ╲ enables the **Line** tool allowing you to 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

This button enables the **Curve** tool allowing you to 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

This button enables the **Polyline** tool allowing you to draw free-form curves
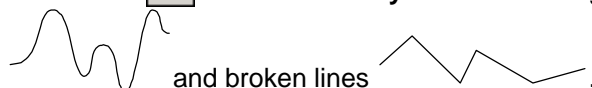
and broken lines .

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

This button enables the **Draw Arrow** tool allowing you to 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 [icon] tool becomes active). If this check box is cleared, the

Select/Move/Resize [icon] tool becomes active immediately after you have drawn an arrow.

4.7.6 Rectangle Button

This button [icon] enables the **Rectangle** tool allowing you to 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 [icon] tool becomes active). If this check box is cleared, the

Select/Move/Resize [icon] tool immediately becomes active after you have drawn a rectangle.

4.7.7 Rounded Rectangle Button

This button [icon] enables the **Rounded Rectangle** tool allowing you to 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 [button image] tool becomes active). If this check box is cleared, the

Select/Move/Resize [button image] tool immediately becomes active after you have drawn a rounded rectangle.

4.7.8 Ellipse Button

This button [button image] enables the **Ellipse** tool allowing you to 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.

> **Note**   To change the thickness, style, and color of a drawn object without affecting defaults, double-click the ellipse 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 [button image] tool becomes active). If this check box is cleared, the

Select/Move/Resize [button image] tool immediately becomes active after you have drawn an ellipse.

4.7.9 Polygon Button

This button [button image] enables the **Polygon** tool allowing you to draw polygons [shape image] and curved

shapes [shape image] .

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.

> **Note**   You can then edit the form of the drawn shape with the help of the **Edit Nodes** [button image] 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.

> **Note**   To change the thickness, style, and color of a drawn object without affecting defaults, double-click the polygon 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 [button image] tool becomes active). If this check box is cleared, the

Select/Move/Resize [button image] tool immediately becomes active after you have drawn a polygon.

4.7.10 Insert Image Button

The **Insert Image** 🔛 button allows you to insert external bitmap images (BMP, JPG, and GIF formats) into the body of a ChemSketch document. 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.

> **Note** 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

This button 🖼 enables the **Text** tool allowing you to insert text at any location on the workspace.

If you click the bottom right triangle of the **Text** 🖼 button, it will be expanded into the following buttons:

🖼 **Formatted Text**

T **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 4.7.11).

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/Rotate ◇ tool.

4.7.12 Table Button

This button enables the **Table** tool allowing you to 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.

Button	Function
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.	
	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.
	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.
	Deletes the column containing a selected cell.
	Deletes the row containing a selected cell.
	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).
	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).
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).	
	Adds a new box for the selected table.
	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..
	Swaps the contents of the selected boxes. Note that you can swap the contents of boxes within one table only.
	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 [ ] to unfold a panel representing various types of brackets:

[ ]	**Brackets**
[	**Bracket**
( )	**Parentheses**
(	**Parenthesis**
{ }	**Braces**
{	**Brace**

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. 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:

The table below lists these common buttons:

Button	Function
Apply	Applies the current panel settings to selected objects.
Update From	Copies the style attributes from the drawn object(s) to the panel. When you click this button, the cursor becomes an arrow labeled **From** ( ). Click the required object to update its style attributes to the panel.
Save...	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 4.11.8.1.
Load...	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.).

4.11.1 Pen Style Panel
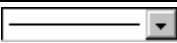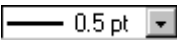
This command displays the **Pen** panel where you can specify the default line style, thickness and color for drawing lines, arcs, arrows, rectangles, ellipses, brackets, and callouts.

> **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.
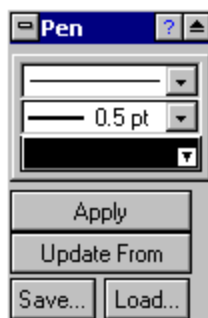
This panel contains the following options:

Option	Function
	In this box, select the line of the needed type.
0.5 pt	In this box, select the line of desired thickness.
	In the color palette, select the needed color for lines.

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:

This panel contains the following options:

Option	Function
☒ **None**	When this button is active, the objects will be drawn with no fill, i.e., they will be transparent.
■ **Solid**	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.
▨ **Pattern**	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.
▦ **Shade**	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.
	In the color palette, choose the needed color.
	In this box, select the needed pattern for hatching.
	In this box, select the required shade type.
Shade -100%	In this box, you can specify the degree of default fill shading, i.e., the percentage of basic color changing in the fill.

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.
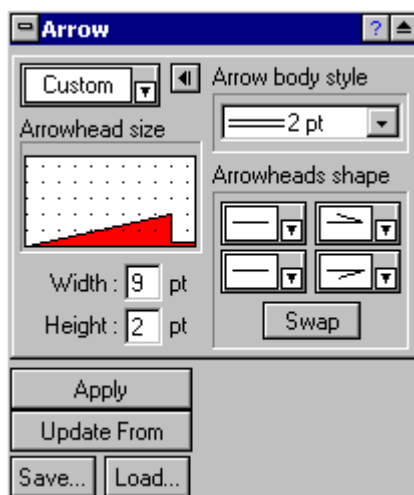
This panel contains the following options:

Option	Function
Custom ▼	In this box, specify the default arrow type. If you choose **Custom**, the panel expands allowing you to specify your own arrow type.
◀	Displays/hides the right part of the panel.
Arrowhead size	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.
Arrow body style	In this box, specify the arrow body type.
Arrowheads shape	In this area, you can specify the default arrowhead shape to be applied to the right and/or to the left arrow ends.
Swap	Interchanges the right and the left arrowheads.

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.
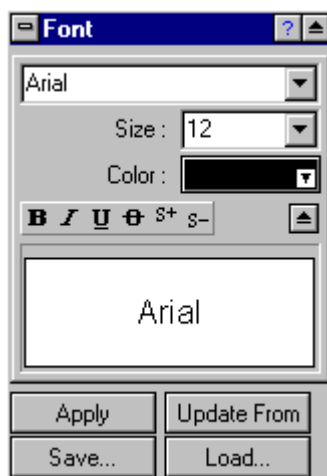
This panel contains the following options:

Option	Function
Style	In this box, you can specify the default font style.
Size	In this box, you can specify the default font size.
Color	In this color palette, you can specify the default font color.
B	Applies **bold** formatting. You can use the bold format button in combination with other options.
I	Applies *italic* formatting. You can use the italic format button in combination with other options.
U	Applies underlined formatting. You can use the underline button in combination with other options.
θ	Applies ~~striked out~~.formatting. You can use the strikeout button in combination with other options.
s+	Sets superscript formatting. You can use the superscript button in combination with other options.
s-	Sets subscript formatting. You can use the subscript button in combination with other options.
▲	Hides/shows the preview area.
Preview area	Shows how characters will look with the options selected. You can hide/display it.

Shortcut:

   Keyboard: CTRL+SHIFT+T

4.11.5 Paragraph Panel
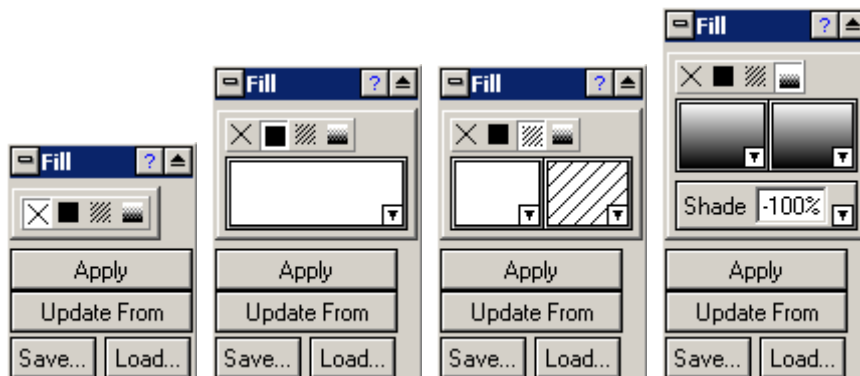
This command displays the **Paragraph** panel where you can specify the default style for paragraphs.

> **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.

This panel contains the following options:

Option	Function
Justification	In this area, specify the alignment for the paragraph by clicking the corresponding buttons: to the left 🗐, centered 🗐, to the right 🗐, and justified 🗐.
Indentation	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**).
Spacing	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.

> **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.

This panel contains the following options:

Option	Function
On the **Box** tab, you can define options for table.	
Use Header	If this check box is selected, the first row in the table is inserted in every box as a header.
Protect Contents	If this check box is selected, the program does not allow you to insert or remove objects from the table cells.
Move to the Right	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.
Move to Next Box	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.
Vertical Justify	If this check box is selected, numbers of rows in each group (column) are approximately equal.

Option	Function
On the **Cell** tab, you can define options for table cells.	
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.
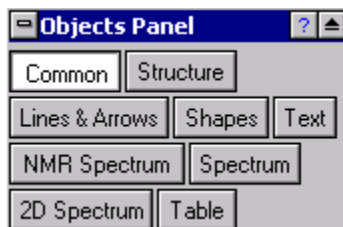
Combine your choices from the tabs and the drop-down lists to create your style, and then click **Apply** to employ changes.
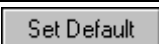
If no objects are selected in the workspace, this command is disabled.

> **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:

The table below lists these common buttons:

Button	Function
Apply	Applies the specified style settings to the selected objects.
Load ...	Displays the list of the available styles. Choose the required style name to load its attributes into the panel.
Set Default	Sets the specified settings as the default.
Save As...	Displays the **Save User Style** 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.

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.
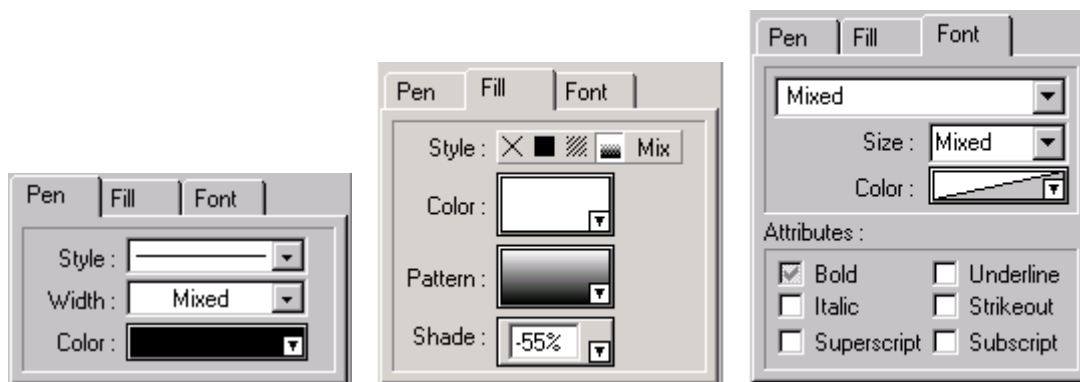
The following options are available:

Option	Function
On the **Pen** tab, you can specify the line thickness, style, and color of the selected objects.	
Style	From the list, choose the line style.
Width	In this box, specify the line thickness for the selected objects.
Color	In this box, specify the line color to be applied to selected objects.

Option	Function	
The **Fill** tab presents options for specifying the fill style, color, and pattern of selected objects.		
Style	In this area, click the required button to:	
	⊠ **None**	Draw the objects with no fill, i.e., they will be transparent.
	■ **Solid**	Draw the objects with the solid fill (you can specify the fill color in the **Color** box that appears).
	▨ **Pattern**	Draw the hatched objects (you can specify the prototype and color for hatching in the **Color** and **Pattern** boxes that appear).
	▨ **Shade**	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, you can specify the fill color to be applied to the selected objects.	
Pattern	In this box, select the needed pattern for hatching or the required shade type.	
Shade	In this box, you can specify the degree of default fill shading, i.e., the percentage of basic color changing in the fill.	
On the **Font** tab, specify the font and paragraph settings for the selected text.		
Style	In this box, you can specify the font style.	
Size	In this box, you can specify the font size.	
Color	In this box, you can specify the font color.	
Attributes	Selecting check boxes applies the corresponding formatting: **Bold** *Italic* <u>Underline</u> ~~Strikeout~~. Superscript (^Superscript^) Subscript (_Subscript_)	

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 the current 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.

The following options are available:

Option	Function
On the **Atom** tab, specify the font options to be used for atom labels of the selected structure(s).	
Font	In this box, specify the font style to be applied to atom labels in the selected structure.
Symbol Size	In this box, specify the font size to be applied to atom labels of the selected structure.
Color	In this box, specify the font color to be applied to atom labels of the selected structure.
Style	In this box, specify the style for atom labels: **bold** and/or *italic*. The pressed-in **Mix** button indicates that the corresponding attribute in the selected objects differs (e.g., the selected structure has some atoms formatted just with bold and some just with italic).
On the **Bond** tab, specify the width and color to be used for bonds of the selected structure(s).	
Width	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 **Preferences** dialog box (**General** tab).
Color	In this box, specify the color to be applied to bonds of selected structure.

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:
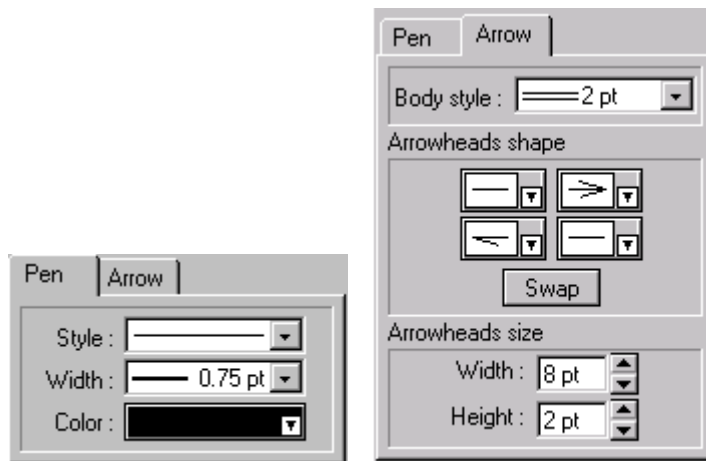
The following options are available:

Option	Function
On the **Pen** tab, you can specify the thickness, style, and color of the line on selected linear objects.	
Style	From this box, choose the line style.
Width	In this box, specify the line thickness for the selected objects.
Color	In this box, you can specify the line color to be applied to the selected objects.
On the **Arrow** tab, you can specify the style of arrowhead and body of selected arrows.	
Body Style	In this box, specify the default arrow body type.
Arrowheads shape	In this area, specify the default arrowhead shape to be applied to both arrow ends.
Swap	Interchanges the arrowheads.
Arrowheads size	In this area, specify the arrowhead width and height.

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:

Option	Function
On the **Pen** tab, you can 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.	
Style	From this box, choose the line style.
Width	In this box, specify the line thickness for selected objects.
Color	In the color palette, you can specify the line color to be applied to the selected objects.
On the **Fill** tab, you can 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:
	⊠ **None** — Draw the objects with no fill, i.e., they will be transparent.
	■ **Solid** — Draw the objects with the solid fill (you can specify the fill color in the **Color** box that appears).
	▨ **Pattern** — Draw the hatched objects (you can specify the prototype and color for hatching in the **Color** and **Pattern** boxes that appear).
	▤ **Shade** — 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, you can 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, you can specify the degree of default fill shading, i.e., the percentage of basic color changing in the fill.

Option	Function
On the **Shadow** tab, you can 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.	
On / Off /Mixed	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).
Color	In the color palette, you can specify the color of the shadow.
dX / dY	In these boxes, you can 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).

4.11.7.5 Objects Panel: Text
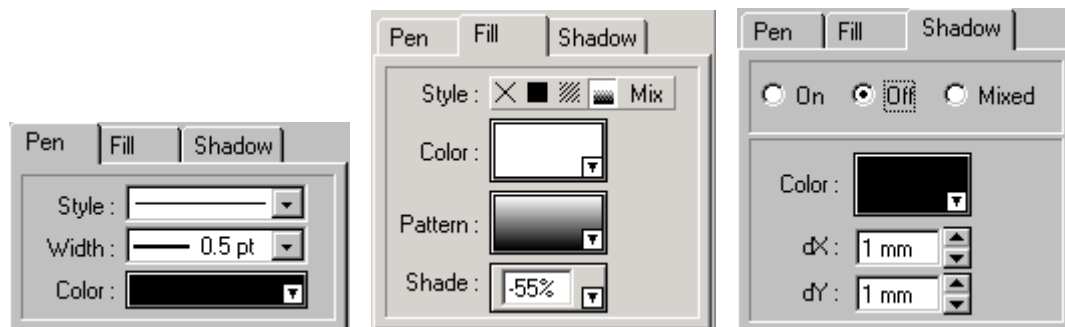
The **Text** button displays tabs with the style settings to be applied to selected text.

The following options are available:

Option	Function
On the **Attr** tab, you can transform the selected formatted text into the artistic one and rotate it.	
Artistic Text	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.).
Angle of Rotation	In this box, you can specify the angle at which you want to rotate the selected text.

Option	Function
On the **Font** tab, specify the font settings for the selected text.	
Style	In this box, specify the font style.
Size	In this box, specify the font size.
Color	In this box, specify the font color.
Attributes	Selecting check boxes applies the corresponding formatting: **Bold** *Italic* Underline ~~Strikeout~~. Superscript (^{Superscript}) Subscript ($_{Subscript}$)
On the **Paragraph** tab, you can specify the style for paragraphs of selected text.	
Justification	In this area, specify the alignment for the paragraph by clicking the corresponding buttons: to the left ☰, centered ☰, to the right ☰, and justified ☰. Text will be aligned relative to the current indents that can be specified in the Indentation area below. The active **Mix** button (Mix) indicates that the justification of the selected objects differs and will not be changed.
Indentation	In this area, you can specify the left and the right indention of the paragraph in the text box as well as the indent of the first line in the paragraph.
Spacing	In this area, 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. 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).

> **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 the current 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 **Preferences** dialog box (**General** 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.

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.

The following options are available:

Option	Function
On the **View** tab, specify the objects to be displayed with the spectrum.	
Spectrum display options	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.
Scale display options	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.
On the **Spectrum** tab, specify the spectrum lines style and labels font style.	
Spectrum Lines Styles	In this area, specify the style, thickness, and color to be applied to the spectrum lines (solute, solvent, and overlapped lines).
Labels Font Style	In this area, specify the style, size, and color for spectrum labels.

Option	Function
On the **Scale** tab, specify the scale line style and label font style.	
Scale Line Style	In this area, specify the style, thickness, and color to be applied to the scale lines.
Scale Font Style	In this area, define the font style, size, and color for scale values.

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:

Option	Function
On the **View** tab, specify the objects to be displayed with the spectrum: labels, integral curves, gridlines, vertical scale, and horizontal scale.	
On the **Spectrum** tab, specify the style for spectrum and scales.	
Spectrum Line Style	In this area, specify the ordinal number of the line for which the style, width, and color should be specified in the **Lines** boxes below.
Scale Style	In this area, define the font style, size, and color for scale values (**Values** boxes), also specify the style, width, and color for scale lines (**Lines** boxes).

Option	Function
On the **Labels** tab, specify the style, position, and orientation of peak labels.	
Labels Style	In this area, specify the style, size, and color for spectrum labels.
Position	In this area, specify the position of peak labels on the spectrum. The selected **Mixed** option indicates that the position of labels in several selected spectra differs and will not be changed.
Orientation	In this area, specify the orientation of peak labels. The selected **Mixed** option indicates that the orientation of labels in several selected spectra differs and will not be changed.
On the **Integrals** tab, specify the styles for integral lines and integral values.	

> **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 the current attribute differs for the selected objects), i.e., this attribute will not be changed for the selected objects.

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:

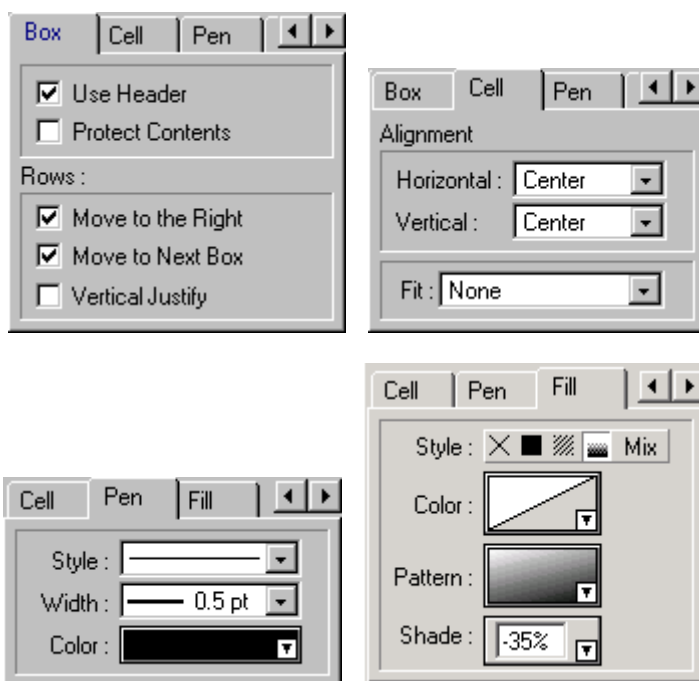| Option	Function
On the **Spectrum** tab, specify the style for 2D spectrum and 1D curves.	
2D Spectrum Colors	In this area, specify the color settings for peaks of the current spectrum and background. As you click the **Coloration Scheme** box, the dialog box appears allowing you to choose the coloration 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.
Plots and **Contours**	In this areas, 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 **Gradient Contour Plot** and **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, and gridlines. 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.
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.

Option	Function
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., the 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:

The following options are available:

Option	Function
On the **Box** tab, specify the general table options including arrangement of table rows in the box in the various ways.	
Use Header	If this check box is selected, the first row in the table is inserted in every box as a header.
Protect Contents	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.
Move to the Right	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.
Move to Next Box	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.
Vertical Justify	If this check box is selected, numbers of rows in each group (column) are approximately equal.
On the **Cell** tab, you can define options for content alignment and manipulation within the 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.
On the **Pen** tab, specify the line style, width, and color of the table borders.	
On the **Fill** tab, specify the fill style and color of table cells.	
Style	In this area, click the required button to:
	⊠ **None** — Draw the objects with no fill, i.e., they will be transparent.
	■ **Solid** — Draw the objects with the solid fill (you can specify the fill color in the **Color** box that appears).
	▨ **Pattern** — Draw the hatched objects (you can specify the prototype and color for hatching in the **Color** and **Pattern** boxes that appear).
	▨ **Shade** — 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, you can specify the fill color to be applied to the table cells.
Pattern	In this box, select the needed pattern for hatching or the required shade type.
Shade	In this box, you can specify the degree of default fill shading, i.e., the percentage of basic color changing in the fill.

> **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 the current attribute differs for the selected objects), i.e., this attribute will not be changed for the selected objects.
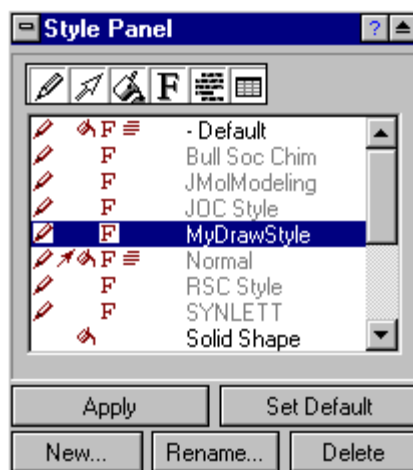
4.11.8 Style Organizer Panel

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:

Option	Function
Attributes	Click the required button to view the styles containing the corresponding attribute. The following attributes are available:
	✎ — **Pen** (for more information on this attribute, refer to Section 4.11.1)
	⬈ —**Arrow** (for more information on this attribute, refer to Section 4.11.3)
	⬥ —**Fill** (for more information on this attribute, refer to Section 4.11.2)
	F —**Font** (for more information on this attribute, refer to Section 4.11.4)
	▤ —**Paragraph** (for more information on this attribute, refer to Section 4.11.5)
	▦ —**Table** (for more information on this attribute, refer to Section 4.11.6)
List of Styles	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.
Apply	Applies the style highlighted in the list to the selected object(s).
Set Default	Sets the style highlighted in the list as the default.
New...	Displays the **Save User Style** dialog box where you can specify the name for your style and to choose the attributes to be included in it. For more information, refer to the section that follows.

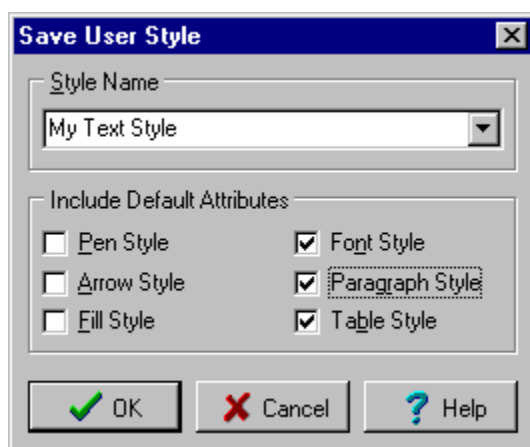| Option	Function
Rename...	Displays the **Rename Style** dialog box where you can specify a new name for an existing style. Note that the built-in styles that appear in gray in the list of styles cannot be renamed.
Delete	Removes the highlighted style from the list. Note that the built-in styles that appear in gray in the list cannot be deleted.

4.11.8.1 Save User Style Dialog Box

In this dialog box, you can specify the 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** Save... or from the **Style Panel** dialog box by clicking **New** New... .

This dialog box contains the following options:

Option	Function
Style Name	Specify a new name for the style or choose the one from the list and modify it.
Pen Style	Select this check box to include current default pen style attributes (specified in the **Pen** panel) in a user-defined style.
Arrow Style	Select this check box to include current default arrow style attributes (specified in the **Arrow** panel) in a user-defined style.
Fill Style	Select this check box to include current default fill style attributes (specified in the **Fill** panel) in a user-defined style.
Font Style	Select this check box to include current default font style attributes (specified in the **Font** panel) in a user-defined style.
Paragraph Style	Select this check box to include current default paragraph style attributes (specified in the **Paragraph** panel) in a user-defined style.
Table Style	Select this check box to include current default table style attributes (specified in the **Table** panel) in a user-defined style.
OK	Click this button to save the specified attributes into the user-defined style with specified name.
Cancel	Click this button to close the dialog box without saving any changes you have made.

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 the current selection.

This command is unavailable if there is only one selected object or no selected objects in the workspace.

Shortcuts:

Keyboard: 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 axis.

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 axis.

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 ![icon] for rotating objects (for more information, refer to Section 4.6.2).
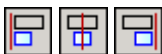
Shortcut:

Editing toolbar: ![icon]

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: ![icons]

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: ![icons]

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** ![icon] 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 3.15.

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 the Command Line

There may be circumstances (such as a call from another program) in which you need to run ACD/ChemSketch from the command line instead of the Windows graphical user interface.

The following command arguments are available to be issued from the command line:

Command	This command…
`chemsk`	Runs ACD/ChemSketch
`chemsk` *`PathFilename.SupportedFormat`* where *`PathFilename.SupportedFormat`* can be a file of any format supported by the current version of ACD/ChemSketch (for the list of supported formats, refer to Section 3.9.8).	Opens the specified file in the ChemSketch window (if possible)
`/print`	Prints the file open in ACD/ChemSketch
`/exportpdf`	Exports the file open in ACD/ChemSketch into PDF format
`/exportpdf:`*`Filename.pdf`*	Exports the file into PDF format with the specified name
`/norestore`	If this switch is added to the command line, all of the specified actions will be executed without opening ACD/ChemSketch
`/quit`	Quits ACD/ChemSketch

> **Note**   The command line length is limited to 260 characters.

For example, the following line:

`chemsk e:\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

`chemsk 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

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 (γ)
- The dielectric constant ε (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 (γ) are founded on well-known physicochemical formula which can be found in literature on physicochemical properties of compounds. They express *d*, *n*, and γ 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 γ 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 γ. These parameters are proprietary information of ACD/Labs, Inc.

The prediction of the dielectric constant ε (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,

$$P_r = \left(\frac{MW}{d} \right) \gamma^{1/4}$$

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, γ

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, ε (Permittivity)

By definition,

$$f(\varepsilon) = f\left(MV, AdditiveFunction\right)$$

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:

$$Polarizability = 0.3964308 \cdot MR$$

## Monoisotopic, Nominal and Average Mass

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.

Correlation Statistics with Experimental Data

Distribution of Molar Refractivity Prediction Error
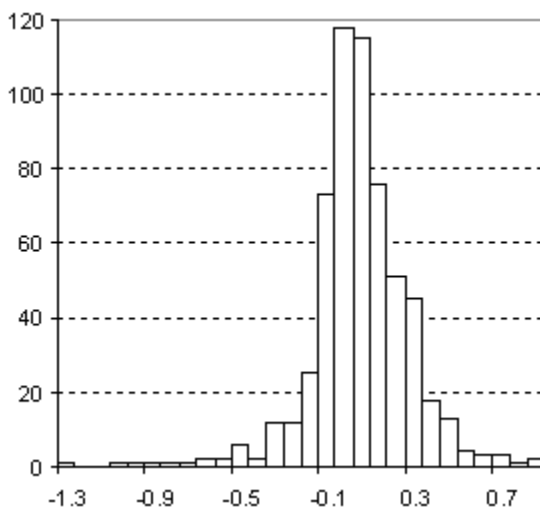
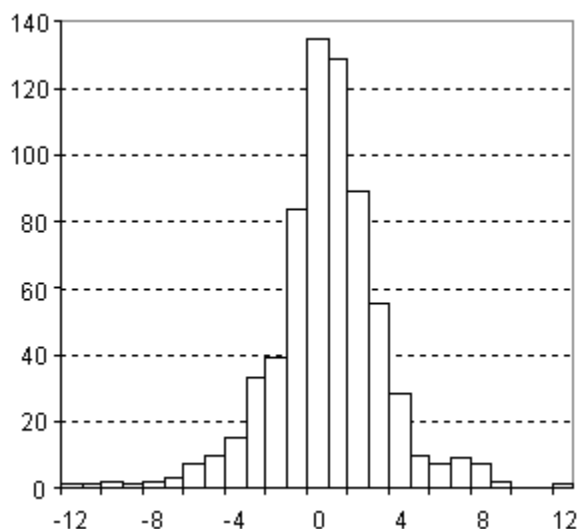| Vertical scale:	Number of Tested Structures
Horizontal scale:	ACD Molar Refractivity Estimation Error
Number of tested structures:	592

$$MR_{exp} = 0.99901(\pm0.00067)\ MR_{calc} + 0.026(\pm0.025) \quad R=0.999867,\ StD=0.23$$

Distribution of Molar Volume Prediction Error

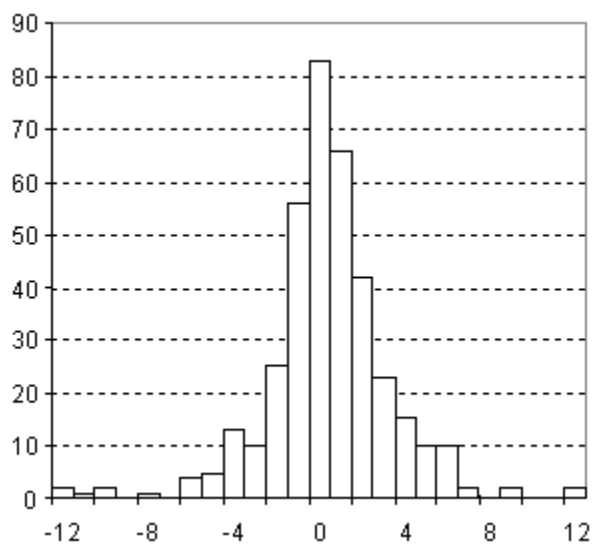| Vertical scale:	Number of Tested Structures
Horizontal scale:	ACD/Molar Volume Estimation Error
Number of tested structures:	671

$$MV_{exp} = 0.9989(\pm0.0020)\ MV_{calc} + 0.18(\pm0.29) \qquad R=0.998626,\ StD=2.74$$

Distribution of the Parachor Prediction Error

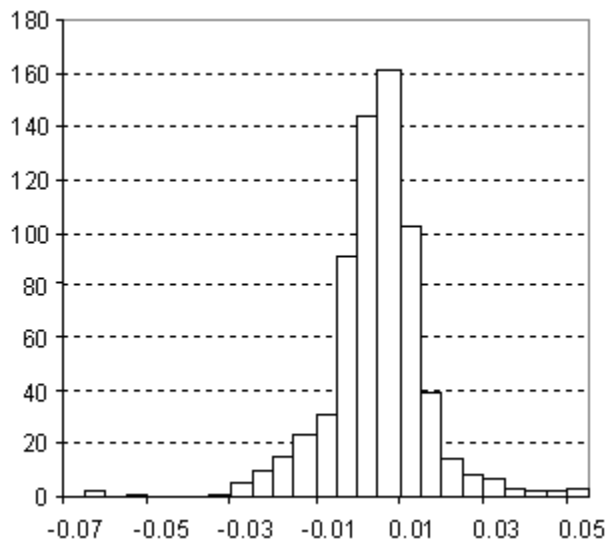| Vertical scale:	Number of Tested Structures
Horizontal scale:	ACD/Parachor Estimation Error
Number of tested structures:	377

$$Pr_{exp} = 0.9978(\pm0.0015)\ Pr_{calc} + 0.68(\pm0.46) \qquad R=0.99958,\ StD=3.11$$

Distribution of the Refractive Index Prediction Error

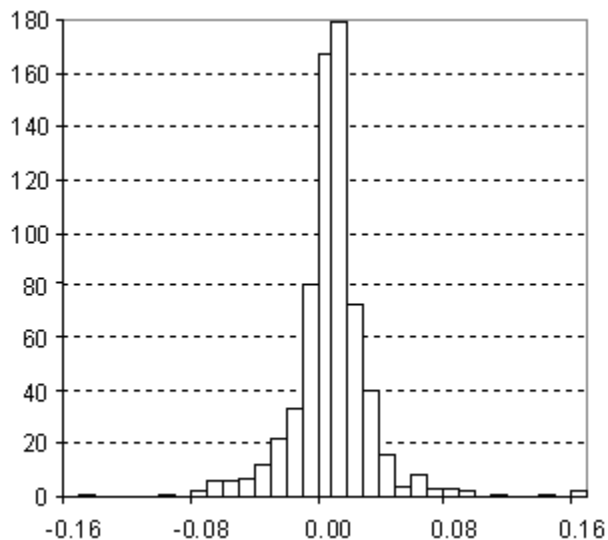|	
Vertical scale:	Number of Tested Structures
Horizontal scale:	ACD/Refractive Index Estimation Error
Number of tested structures:	665

$$n^{20}_{exp} = 0.98035(\pm0.0073)\, n^{20}_{calc} + 0.028(\pm0.011) \qquad R=0.982,\ StD=0.012$$

Distribution of the Density Prediction Error

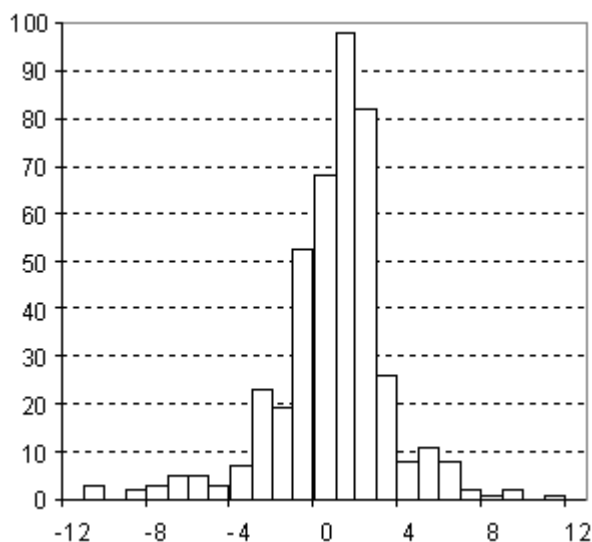|	
Vertical scale:	Number of Tested Structures
Horizontal scale:	ACD/Density Estimation Error
Number of tested structures:	671

$$d^{20}_{exp} = 0.9947(\pm0.0036)\, d^{20}_{calc} + 0.0052(\pm0.0036) \qquad R=0.995683,\ StD=0.028$$

Distribution of the Surface Tension Prediction Error

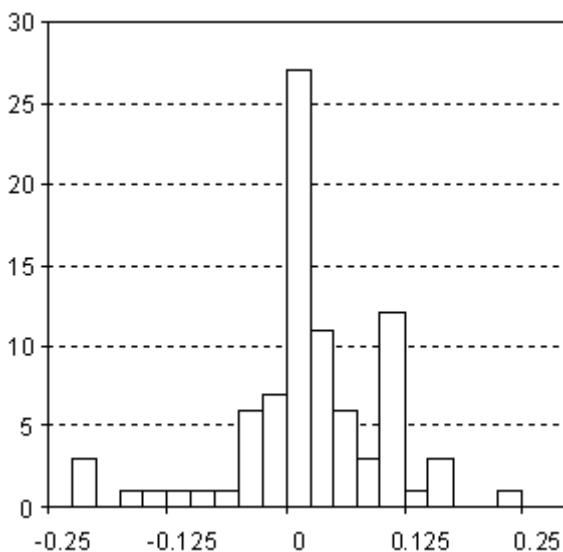|	
Vertical scale:	Number of Tested Structures
Horizontal scale:	ACD/Surface Tension Estimation Error
Number of tested structures:	432

$$st^{20}_{exp} = 0.998(\pm0.018)\ st^{20}_{calc} + 0.08(\pm0.53) \qquad R=0.934720,\ StD=2.84$$

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
	Note: Derived only for hydrocarbons

$$\varepsilon_{exp} = 1.005(0.033)\varepsilon_{exp} - 0.013(0.072) \qquad R=0.9588,\ StD=0.079$$

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?

To check if you already have Goodies, look for all .BAS files within your ACD/Labs example folder (\\EXAMPLES\CHEMBAS\GOODIES). If you don't find any, you can download them from our Web site free of charge at

http://www.acdlabs.com/products/chem_dsn_lab/goodies.html

They are easy to install and to use. Just follow the installation instructions provided at the aforementioned Web page and enjoy these new ACD/ChemSketch features.

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

Below is the list of Goodies tools that are available at the moment at our Web site:

Goodies	Function	How to use
Insert Page	Inserts 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.	Go to the page before which you want to insert a blank page and click **Insert Page**.

Goodies	Function	How to use
Clone Page	Clones 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.	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	Moves and copies pages—*i.e.,* changes page order in your document.	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	Allows you to cut-and-paste or copy-and-paste a sequence of pages to a new position within the same document.	Click this button 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	Deletes a range of pages at a time. Note that the pages you have deleted cannot be recovered with the **Undo** command from the **Edit** menu.	Click **Delete Pages** . In the dialog box that appears, type the sequence of pages to be deleted and click **OK**.
Rename Pages	Changes the name of pages. Note that the names of the pages will be shown when you click **Page 1/1** on the status bar.	Click this button 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**.
Insert Page Numbers/ Annotations	Inserts page numbers or complex annotations in your document. Note that an annotation will be inserted at the bottom right corner of the page.	Click this button 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)) 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.

Goodies	Function	How to use
Annotate Document	Annotates 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.	Click this button 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 Browser	Looks through the folders to find the specified ChemSketch documents as well as to search ChemSketch documents for the text string without opening them.	Click this button and follow the instructions that appear in the dialog box.
Create HTML	Exports all the 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.	All the details may be found in FILLTMP.DOC file provided in the Goodies folder (\\EXAMPLES\CHEMBAS\GOODIES).
Sketch-to-VRML Converter	Exports all of the structures from the current page into a VRML 2.0 file, which you may then view with Cosmo, GLView, or any other VRML browser.	Draw structures which you wish to export on the same page, and then click this button. In the dialog box that appears, type the name and location of .WRL file to which structures are to be exported. Note that 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	Imports the data (structures, text, *etc.*) from a file of MDL's SDfile format into ChemSketch document.	Click this button 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	Exports all of the structures from the current page or from the whole document to an SDfile	Open the page with the structures you want to export (if required). Click this button 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.)

Goodies	Function	How to use
Table Wizard	Creates tables or/and aligns objects according to the specified number of rows and columns.	Click this button; 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	Replaces 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 that this can only be done with a single structure on the page.	Draw or leave only one structure on the page and click this button. 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 that the hydrogen atoms should be drawn explicitly (use **Add Explicit Hydrogens** from the **Tools** menu).
Solution Calculator	Calculates the weight of a compound required for preparing an aqueous solution of the user-defined volume and molar concentration. Note that program execution is possible only with a single structure on the page.	Draw or leave one structure on the page and click this button. In the dialog box that appears, specify the required molar concentration and aqueous solution volume, then click **OK**.
Label Printer	Quickly creates labels for chemicals and prints them according to the Avery Standard (45 templates included) or according to your own template.	Draw structures for which you want to create labels and click **Label Printer**. Note that you can create labels for structures from an SDfile if you run this program with an empty active page. For more information, see LPRINTER.TXT provided in the Goodies folder (\\EXAMPLES\CHEMBAS\GOODIES).
Peptide Builder	Builds a 3D peptide structure from the amino acids sequence.	Refer to the PEPBUILD.SK2 file provided in the Goodies folder (\\EXAMPLES\CHEMBAS\GOODIES) as a guide to using this tool.
Carbohydrate Builder	Builds a structure from carbohydrate abbreviated names.	For information on how to work with this tool, refer to the SUGARSK.TXT file that you can find in the Goodies folder (\\EXAMPLES\CHEMBAS\GOODIES).
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.)	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.

Goodies	Function	How to use
Nucleic Acid Builder	Builds a 3D nucleic acid (DNA, RNA) structure (one or two chains) from your input sequence.	Click this button 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.	Click this button 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.)