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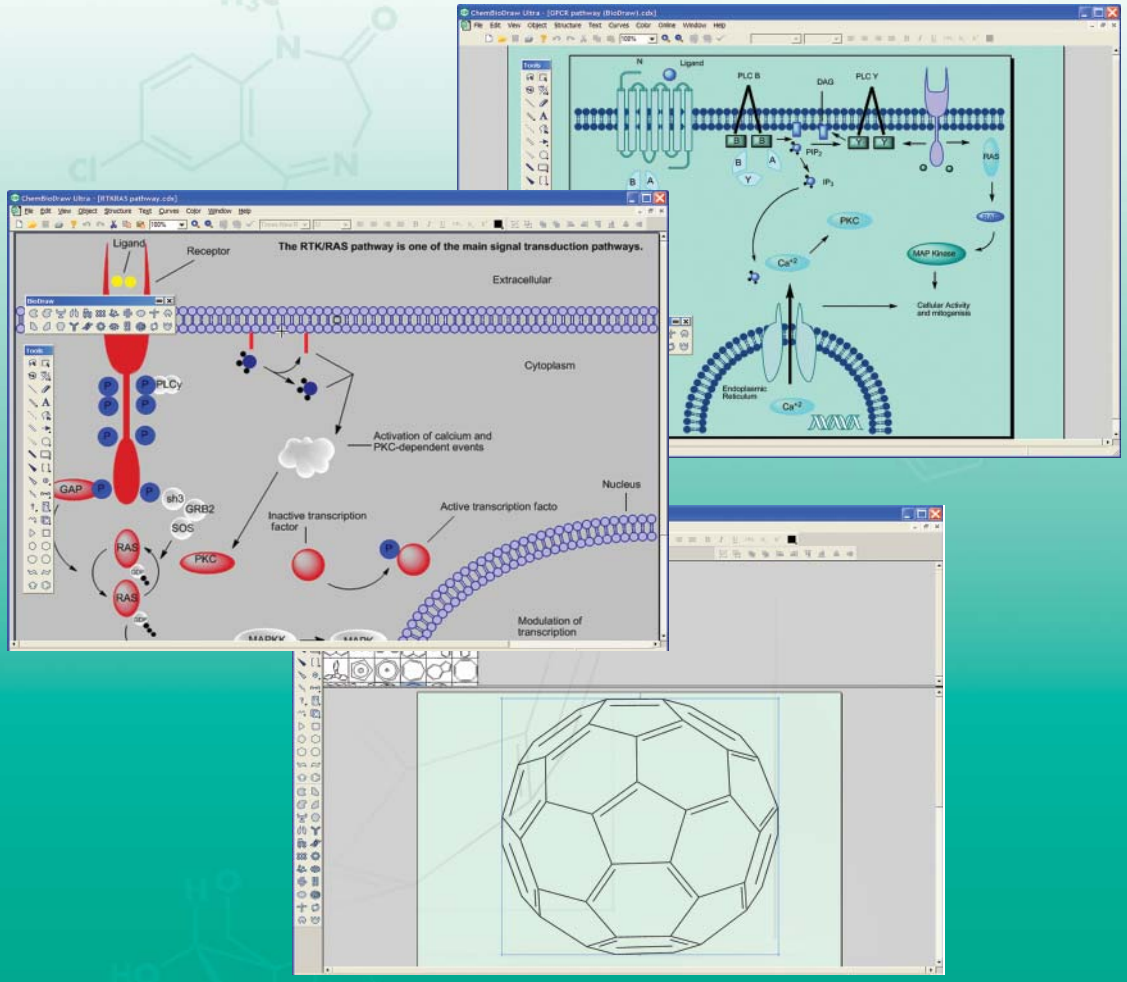


Chem & Bio Draw®

Chem & Bio Drawing Standard

Contents

1

Getting Started

This section will help you become familiar with the ChemDraw user interface.

The Toolbars

The toolbars in Chem & Bio Draw 12.0 provide all the tools necessary to draw and edit structures.

The Main Toolbar

Most common tools are on the main toolbar. These include all the bond, shape, text, and selection tools necessary for drawing structures and reactions. Other toolbars, such as the arrow toolbar, may be activated from the main toolbar.

The Symbols Toolbar

You can activate the symbols toolbar from the main toolbar. Use the symbols to represent cationic and ionic charges, radicals, and lone electron pairs in your structures

The Arrows Toolbar

Use arrows to draw reactions or to add simple annotations to your drawings.

The General Toolbar

This toolbar provides several miscellaneous but valuable control tools. Use this toolbar to zoom in and out on objects, undo you last change, clean up structures, and color objects. You can also activate the online help if you need assistance with any of the available tools.

Periodic Table

Use the periodic table to insert atoms into structures. Go to **View**>**Show Periodic Table Window**.

Click a symbol to highlight the atom and activate the Text tool. Drag across the table to highlight each atom.

TO ADD AN ATOM

Select it in the periodic table and click an empty space in the document. The atom appears in its chemically neutral form. For example, carbon appears as CH_4 and hydrogen appears as H_2.

TO LABEL AN ATOM

Click an existing unlabeled atom.

TO CHANGE THE OXIDATION STATE

Using the symbol for the atom, click the atom in the document window.

TO CHANGE TO A DIFFERENT ATOM

Select the new atom in the periodic table and click the atom in the document you want to change.

TO EDIT A LABEL

To modify the atom label, double-click the atom in the document window.

NOTE: Some element names conflict with ChemDraw 12.0 Hotkeys and may not be interpreted correctly.

2

Basic Drawings

ChemDraw 12.0 provides a variety of tools for drawing everything from simple chemical structures to complex reactions. In this section, we introduce basic drawing techniques to help you create your first structures. We also explain how to add features such as arrows and shapes to enhance structures and reactions.

Bonds

The Main toolbar offers numerous options for drawing bonds. Some of the tools are for drawing specific types of bonds while others represent nonspecific bonds for drawing structures for database queries.

Drawing bonds

All bonds that you draw are, by default, constrained to a fixed length and fixed angle. To draw the first bond of your structure, select the solid bond tool in the Main toolbar and click in the document window. To draw another bond, click either end of the first bond.

Figure 2.1 Adding a bond to an atom

You can draw a bond in any direction. Using a bond tool, click and drag from an existing atom or an empty area in the document window. The bond is drawn in the direction you drag the cursor.

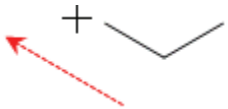


Figure 2.2 Adding a bond by dragging

Bond Types

Double Bonds

There are two ways to draw a double bond:

- Draw a bond using the Double bond tool.
- Draw a single bond over an existing single bond.

Wedged Bonds

Wedged bonds are drawn with a fixed orientation in a document window.

To draw a wedged bond:

1. Click one of the wedged bond tools.
2. Drag from the narrow end of the wedged bond to the wide end of the wedged bond.

- To change the orientation of the wedged bond, click the center of the bond using the wedged bond tool.

NOTE: ChemDraw 12.0 treats hashed wedged bonds with the narrow end in the plane of the screen and the wide end behind the plane.

Editing Bonds

You can modify the appearance of chemical bonds by:

- Changing bond types
- Changing bond alignment and orientation
- Moving Atoms
- Layering bonds

Changing Bond Types

Change a bond from one type to another selecting a bond tool and clicking the center of an existing bond.

Aligning Double Bonds

Double bonds can have one of three alignments relative to other bonds— above, below, and centered.

Above	
Below	
Centered	

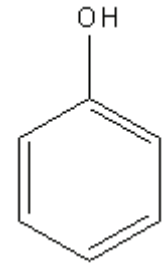
1. Click the bond tool used to create the existing double bond.
2. To change the alignment, click the center of the double bond.

Moving Atoms

1. Click a selection tool.
2. Point to the atom to move. A highlight box appears over the atom.
3. Shift+drag the atom.

Atom labels

You can annotate simple hydrocarbon structures using atom labels using the text tool. For example, you can add the atom label “OH” to create:



1. Using the Benzene tool, click in the document window. A benzene ring appears.
2. Using the Solid Bond tool, click one of the benzene carbons to create toluene.
3. Using the Text tool, click the end carbon on the methyl group of toluene. A text box appears.
4. In the text box, type OH.
5. Click outside the text box.

To edit the atom label, click in the text box with the text tool and begin typing.

Deleting Labels

To delete an atom label, leaving the underlying bonds unchanged, do one of the following:

- Select the Eraser tool and click the atom label.

- With a selection, bond, or ring tool selected, point to the atom label and press the spacebar, Backspace, or Delete key.

Using Nicknames

Using Nicknames, you can add short names for functional groups to use as an atom label or part of a label. When you label an atom with a nickname, the expanded structure retains its chemical significance.

Commonly used nicknames, such as Me, Et, and Ph are stored in your ChemDraw Items folder. You can edit this list within the GUI (however, you should not attempt to edit this file directly).

Applying Nicknames

You may type a nickname into your structure.

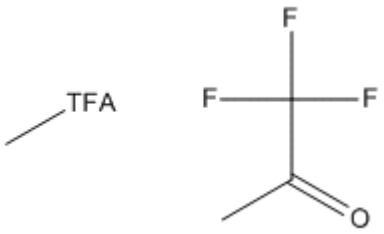
To type the nickname:

1. Double click an atom with a bond tool or click an atom with the Text tool.
2. Type the nickname in the text box.

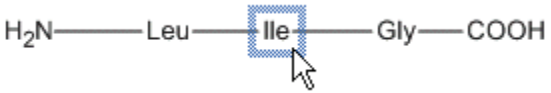
NOTE: Nicknames are tokens and do not flip orientation when applied to the left side of a structure when using Automatic Justification. For example, in the absence of a defined Nickname, the label "OTHP" appears as "PHTO". However, since the Nickname "THP" is defined, the label appears as "THPO".

Expanding Nicknames

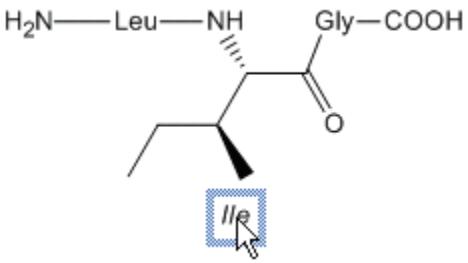
A nickname is a type of label. Therefore, you expand and contract nicknames the same way. When you expand a nickname into its structure, the nickname itself disappears (unless the nickname represents an amino acid or nucleic acid). Trifluoroacetone is shown here:



You can use nicknames to select and help you modify the functional groups they represent. For example, assume you have a chain of three amino acids– glycine, isoleucine, and leucine:



After you expand the nicknames, you can select any of the amino acids by double-clicking its nickname, as shown:



To contract nickname, go to **Structure**>**Contract Label**.

Rings

You can draw aliphatic and aromatic rings of different sizes and types.

1. In the Main toolbar, select a ring tool.
2. Click and drag in the document window to orient the ring.

If you click an atom or bond with a ring tool in an existing structure, the ring is fused to it.

Aromatic Structures

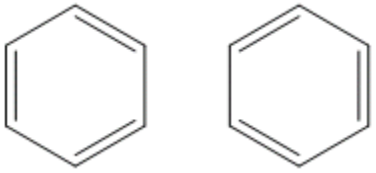
Delocalized rings

You can draw a resonance delocalized ring using any ring tool except for the cyclohexane chairs.

1. Click a ring tool.
2. Press the **Ctrl** key and drag or click in the document window.

Resonance structures

You can draw benzene in either of its two orientations:



To draw, click in the document window with the benzene drawing tool. To draw a different orientation, Shift-click in the drawing window.

Arrows and Shapes

Use the tools and tool palettes on the main toolbar to add shapes to your documents (A tool palette is indicated on the main toolbar by an arrow). You can tear off the palettes and place them where you want.

Objects, except for daggers and some symbols, can be rotated and scaled.

Arrows

You can customize arrows not only for length and angle, but for arrowhead width and shape. You can also drag an arrow from its middle to create an arc of any length.

When you mouse-over an arrow with the Lasso, Marquee, or an Arrow tool selected, the application switches to edit mode and adjustment handles appear on the arrow.

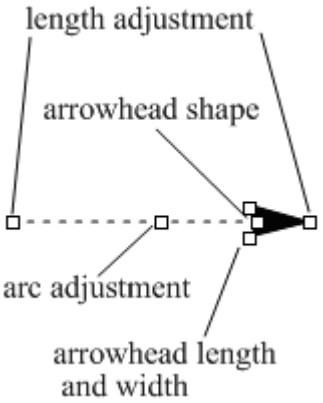


Figure 2.3 Arrow adjustment handles

Drag the adjustment handles to change the arrow length, angle, or shape. When changing the angle of an arrow, you are restricted to multiples of 15° if the **Fixed Angles** is selected. Hold down the **Alt** key to drag to any angle.

The Bracket Tools

These include brackets [ ] and parentheses ( ).

Paired Brackets

Paired brackets can only be placed in a vertical orientation. A rectangle or box defines their position.

To draw a paired brackets:

1. Select a paired bracket tool from the Drawing Elements palette.
2. Point where you want a corner of the bracket.
3. Drag from one corner of the box diagonally to the opposite corner.

Selecting Objects

Use the Lasso or the Marquee tool to select any object. You use the Lasso for freehand selection and the Marquee to select rectangular regions.

To set one selection tool to behave like the other, click the Lasso or Marquee tool while holding the **Alt** key down.

To toggle a selection tool and the last drawing tool used, press **Ctrl+Alt+Tab**.

If you haven't used either selection tool, it defaults to the Lasso tool.

When you select a structure or object, the selection is displayed with a light blue frame around it with three types of selection handles. with a resize handle on each side and corner.

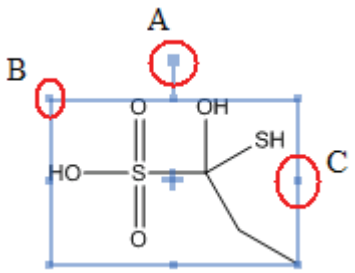


Figure 2.4 A) Drag this handle to rotate the object; B) Drag any corner to resize; C) Drag any side handle to distort.

The Lasso Tool

Use the Lasso tool to make freehand selection of irregular areas.

To select objects using the Lasso tool:

1. Select the Lasso tool.
2. Press the mouse button while the pointer is not over any object.
3. Drag around part of a structure or other object.

As you drag, a line appears that defines the selection area. Bonds, structures, or other objects are selected only if they are entirely within this area. The end points of the Lasso are connected when you release the mouse button.

The Marquee Tool

Use the Marquee tool to select objects and structures within a rectangular area.

1. Select the Marquee tool.
2. Click and drag diagonally over the structures or other object.

As you drag, a rectangle appears that defines the selection area. Bonds and other objects are selected only if they are entirely within the rectangle.

Selecting entire structures

To select an entire chemical structure, double-click a bond or atom in the structure using a selection tool.

If the chemical structure or other object is part of a group, the group is selected.

Selecting objects by clicking

1. Select the Lasso or the Marquee tool.
2. Point to an object in a document window.

A highlight box appears over the selected object. If you point at a bond, the highlight box appears over the length of the bond.

3. Click the object.

The selected objects appear within the Selection Rectangle and the cursor changes to a hand.

Selecting multiple objects

When you select multiple objects, each object displays a selection box, so that you can see exactly what is chosen.

To add more objects to the selection, press **Shift** and select the other objects.

To select all objects, go to **Edit**>**Select All**.

Deselecting all objects

To deselect all objects, do one of the following:

- Click an empty area outside the selection rectangle.
- Press **Esc**.
- Select a different tool.
- Select another object without holding down **Shift**.

Deselecting one object

To deselect only one of several selected objects, hold down the **Shift** key and click the object with a selection tool.

NOTE: As shown in the figure below, objects may appear within the borders of the selection rectangle but not be selected.

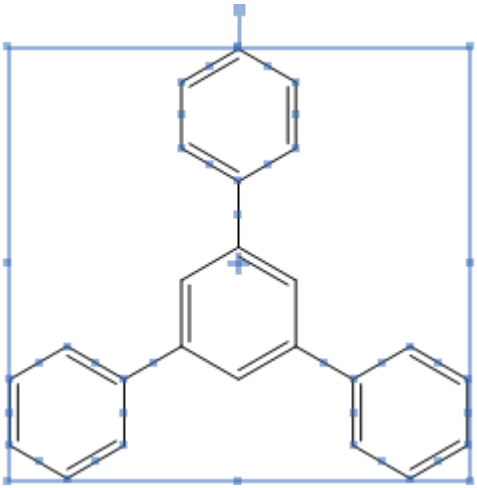


Figure 2.5 Removing selected objects. Blue dots on the surrounding rings indicate these rings have been selected. The center ring has not been selected.

Resizing Objects

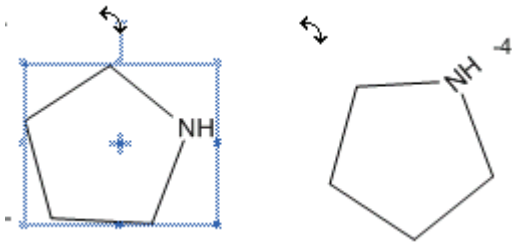
To resize a selected object, click and drag a handle.

- resize proportionately by dragging any corner.
- resize with either X-axis or Y-axis distortion by dragging any side.
- resize freely (X and Y axis distortion) by holding the **Shift** key down while dragging.

Rotating Objects

1. Select an object to rotate. The Rotation handle is at the top of the selection rectangle.
2. Drag the Rotation handle clockwise or counterclockwise.

To rotate an atom label with a structure, press the **Ctrl** key while dragging the structure.



NOTE: If an atom is unselected when a structure is rotated, the structure rotates around the unselected atom.

Moving Objects

1. Select an object to move using a selection tool.
2. Click and drag the object to a new location.

To constrain the movement to the horizontal or vertical direction, **Shift+drag** the selected objects.

Small incremental movements are often useful for aligning objects.To move an object a incrementally:

1. Select the object.
2. Press an arrow key. The selected object moves 1 point in the direction of the arrow.

NOTE: To move in a larger increment, hold down the **Alt** *key while dragging the object. The selected objects move 10 points in the direction of the arrow.*

Moving Atoms

You can move an atom in a chemical structure, click and drag it using a selection tool. The bonds connected to the atom stretch.

To move multiple atoms, select only the bonds that have atoms on both ends that you want to move. The unselected bonds attached to the selected atoms are stretched.

NOTE: You can also move atoms using the bond tool used to draw the atom. See "Moving Atoms" on page 4.

Copying Objects

1. Select one or more objects.
2. **Ctrl+drag** the object(s) to create a copy and position it.

To constrain the copy to move only vertically or horizontally while positioning it, hold down the **Shift+Ctrl** keys.

Deleting Objects

To delete selected objects, press the **Delete** key.

3

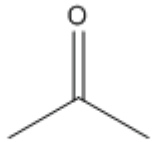
Tutorials

Overview

The tutorials illustrate fundamental drawing techniques. Each tutorial introduces new techniques, or variations of techniques learned in previous tutorials. We therefore suggest that you follow the tutorials in order.

Tutorial 1: Drawing a Structure

In this tutorial, we explain how to draw the structure below:



2-propanone

To create the bonds:

1. On the main toolbar, select the Solid Bond tool.
2. Position the cursor (+) anywhere in the document window and click. A bond appears.
3. To add a second bond, click the right-end of the bond you just created.

Figure 3.1 Attaching a bond to an existing bond

4. To create a tertiary carbon, click in the same place as you did in step 3.

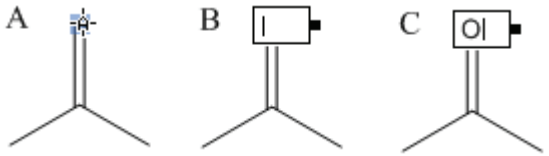
Figure 3.2 Adding a third bond

CHANGING BOND ORDER

To create the double bond, either click and drag over the vertical bond you drew in step 4 or simply double-click it.

Figure 3.3 Adding a double bond

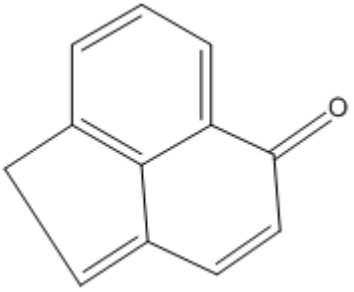
1. Using the Text tool, click the end of the double-bond shown below. A text box appears at the end of the bond.



2. Type an uppercase **O** in the text box.
3. Close the text box by either pressing the Esc key or choosing another tool.

Tutorial 2: Using Rings

In this tutorial you use rings to create the structure below:



Create the ring system:

1. Click the **Benzene** tool.
2. Shift-click in an empty area of the document.

> *NOTE: Hold down the shift key to change resonance structures when using the cyclopentadiene or benzene tools.*

3. Point to the center of the lower right bond in the benzene ring.
4. Click to fuse another ring.

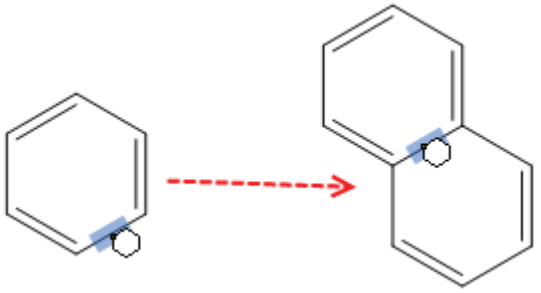


Figure 3.4 Fusing rings

5. In the final structure, there is supposed to be only one double bond in the second ring. To correct the current structure, click one of the double bonds using the Single Bond tool. Do the same for the other double bond.

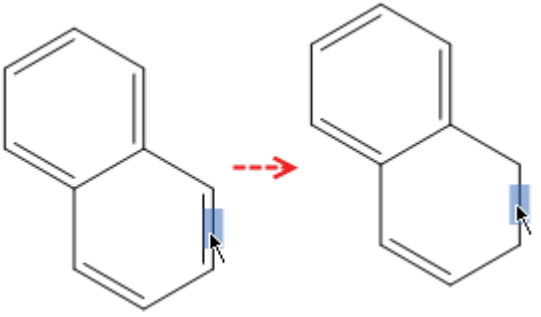
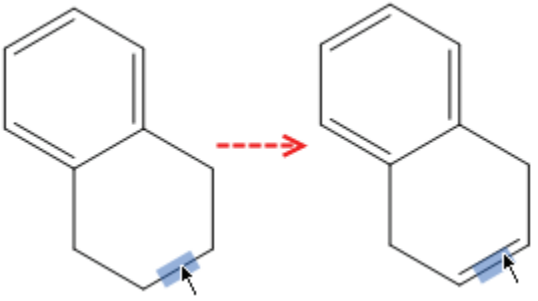
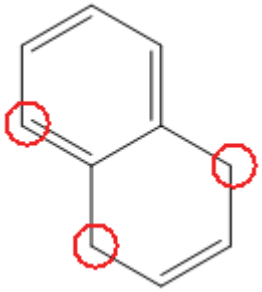


Figure 3.5 To change the bond order, type '1'.

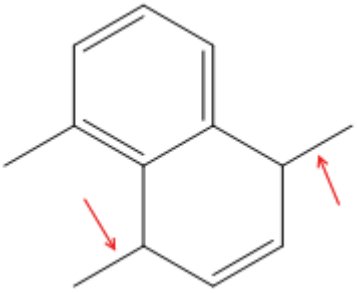
6. To create the double bond in the second ring, click it using the Double Bond tool.



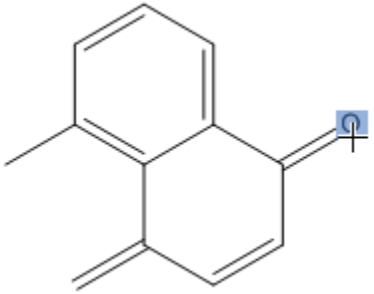
7. Using the Single Bond tool, click the carbon atoms circled in the figure below. Three new bonds will appear.



8. Using the Double Bond tool, click the bond shown below. Do the same for the other bond.



9. Double-click the right-most terminal carbon and type the letter **O** to create the ketone functional group.



10. To connect the left terminal carbons, select the solid bond tool and click-drag a bond from one carbon to the other.

The structure is complete.

Tutorial 3: Fischer Projections

This tutorial demonstrates creating a Fischer projection of glucose (shown below).

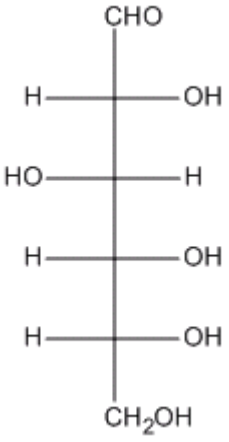


Figure 3.6 Fischer projections

To draw the first bond:

1. Click the Solid Bond tool.
2. Point in the document window. Drag downward vertically to draw the first bond.
3. Point to the lower atom, and drag downward again to draw the second bond.

The red wavy box appears because Show Chemical Warnings is selected. We will keep it selected for now.

4. Repeat step 3 three more times to draw a total of five bonds.

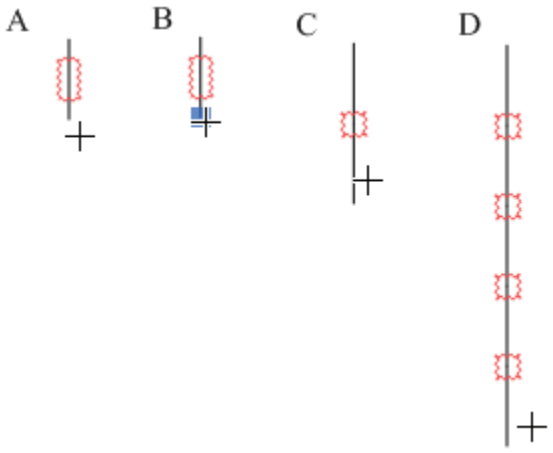


Figure 3.7 Drawing the backbone

NOTE: When you drag the pointer along the length of the bonds, the pointer alternates between an arrow and a cross. The arrow indicates you are pointing over the center of a bond, and the cross indicates you are pointing to an atom.

Add horizontal bonds to the second atom in the string of bonds you created:

1. To add a perpendicular bond, point to the uppermost Chemical Warning box and click it.

Note that the red wavy box disappears as soon as you add a bond.

2. Click again to add a horizontal bond in the opposite direction.
3. Repeat steps 1 and 2 with each successive Chemical Warning box until all horizontal bonds are added.

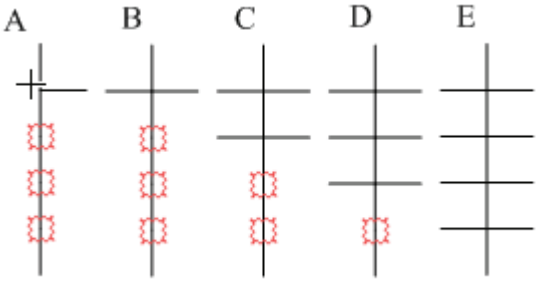


Figure 3.8 Adding horizontal bonds to the backbone

Add labels to the first and last carbon atoms:

1. Select the Text tool.
2. Double-click the uppermost carbon atom to create a text box, and type **CHO** in uppercase.
3. Double-click the lower-most carbon atom, and type **CH2OH** in uppercase.

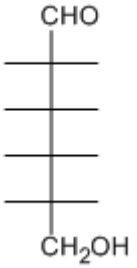


Figure 3.9 Adding atom labels

Add the repeating labels for the hydrogens and hydroxyls:

1. Double-click the atom shown in *A* below and type **H** in uppercase.

2. Double-click each of the other atoms labeled as hydrogen in *B*.

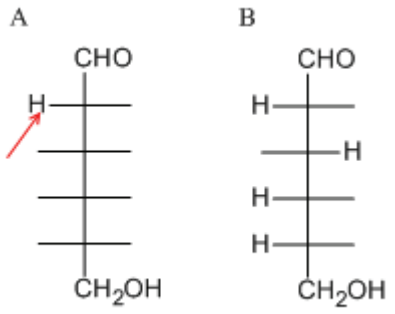


Figure 3.10 Adding repeating atom labels

TIP: Double clicking with the text tool repeats the last label.

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3. Click one of the remaining atoms and type **O** in uppercase.
4. Double-click the remaining atoms to repeat the label.

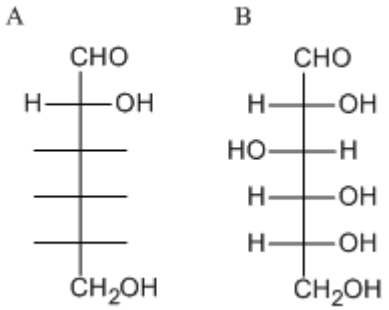


Figure 3.11 Completing the drawing

Tutorial 4: Perspective Drawings

In this tutorial, we explain how to create a perspective drawing by creating a model of α–D–glucose as a Haworth projection.

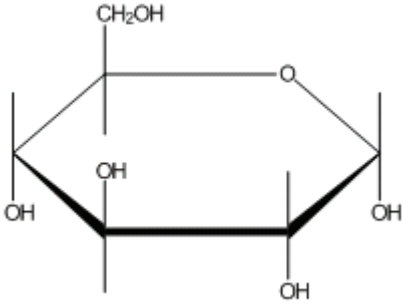


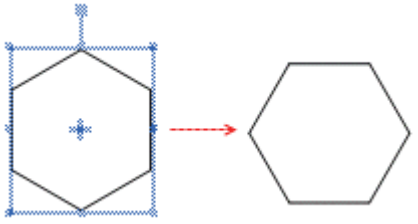
Figure 3.12 Perspective drawings

Draw a ring:

1. Click the Cyclohexane Ring tool.
2. Click in an empty area of a document window. A cyclohexane ring appears.

Rotate the ring:

1. Use the Lasso or Marquee tool to select the ring.
2. Click and drag the rotate handle to rotate the ring 30 degrees.



Change cyclohexane to tetrahydropyran:

1. Click outside the structure to deselect it.

2. Point to the atom indicated in the figure below, and type the letter **O** in uppercase.

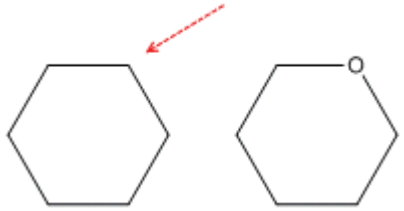
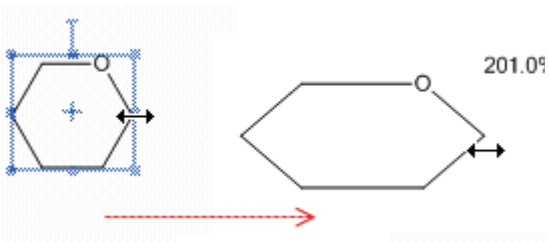


Figure 3.13 Adding an atom label with a HotKey

Resize horizontally:

1. Go to **Edit**>**Select All** (or type **Ctrl-A**).
2. Using a selection tool, click-drag the right side handle to resize the ring horizontally. Release the mouse button when the ring is stretched about 200%.

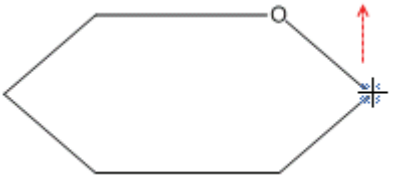


Resize the ring:

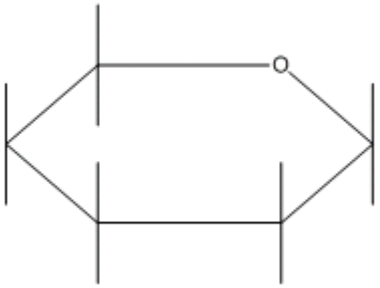
1. Go to **Edit**>**Select All** (or type **Ctrl-A**).
2. Click-Drag the ring a corner adjustment handle increase the size of the ring to 150%. A dialog box appears, asking you whether you want to scale the drawing and text settings.
3. In the dialog box, click **No**.

Add vertical bonds:

1. Click the Solid Bond tool.
2. Point to the atom shown in the figure below and drag upward to create a bond.



3. Point to the same atom, and drag downward to create another bond.
4. Repeat this procedure four more times, adding the pairs of vertical bonds shown below:



Create OH labels:

Point to where you want the label and type **O** in uppercase. You can also use the Text tool method described in the steps below.

1. Select the Solid Bond tool, point to the atom shown in the figure below and double-click to open a text box.

2. Type **OH**.

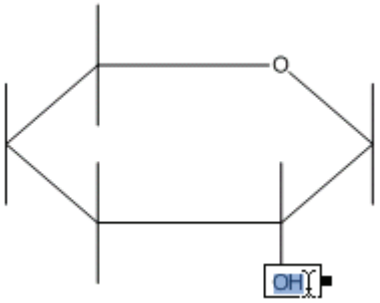
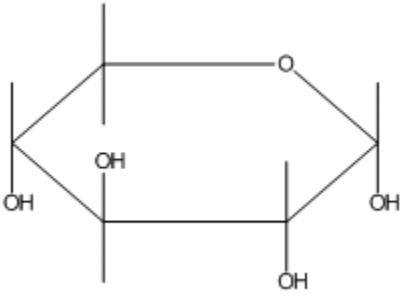


Figure 3.14 Adding the OH labels

3. Move the pointer to the other atoms as shown, and triple-click to repeat the atom label.



TIP: If placing the labels is difficult because of the drawing size, go to **View**> **Magnify**.

Add the CH_2OH label:

1. Triple-click the upper atom of **C5**.

2. Press the Enter key to open the atom label text box. Type **CH2** before the OH.

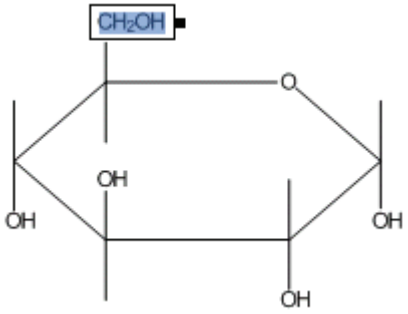


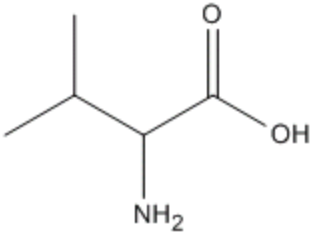
Figure 3.15 Adding the CH_2OH label

NOTE: When used with a bond tool active, Enter *is a Hotkey that opens a text box for the last atom labeled.*

Tutorial 5: Stereochemistry

This tutorial demonstrates using Stereochemistry markers and the flip command. As you draw the structure below, you may notice that some of the steps are similar to those needed earlier to draw isobutane.

First, we draw the following structure:



2-amino-3-methylbutanoic acid

Drawing the structure

To draw the structure:

1. Click the Solid Bond tool.

2. In the document window, click and drag downward to create the first bond.
3. Point at the lower atom and click to add a second bond.
4. Continue pointing at the same atom and click again to add a third bond.

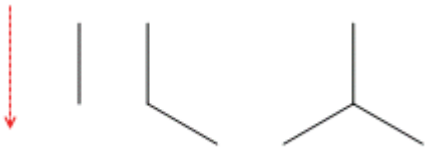


Figure 3.16 Creating the initial structure

5. Point to the atom shown in the figure below and click twice to create two more bonds.

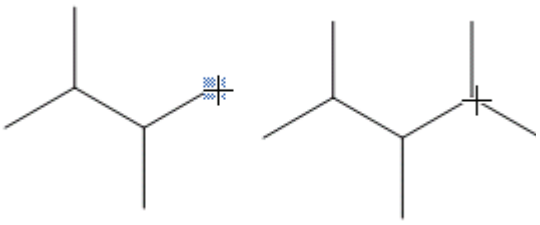
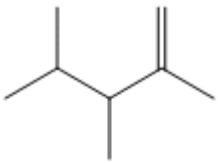


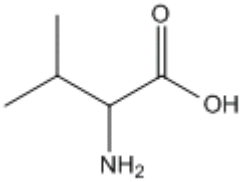
Figure 3.17 Repeating the bond sprouting

Now, turn the single bond at the upper right into a double bond using any of the methods described in the earlier tutorials.



Adding Atom Labels

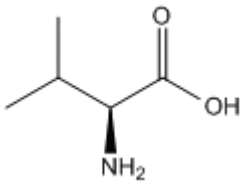
1. Double-click the alpha carbon atom and type **NH2** in the text box that appears. Press the **Esc** key when finished.
2. Add the O and OH with the text box.



Adding Stereochemical properties

We now add stereochemical properties to the structure. First, we change the carbon-nitrogen bond to a solid wedge bond

To add the solid wedge, point to the carbon-nitrogen bond, select the Wedge Bond tool, and click the bond.



4

Advanced Drawing Techniques

The advanced features in ChemDraw are designed to either help you save time or to perform functions that simply can't be accomplished using the basic tools. For example, you can see your drawing as 3D models or create stereoisomers at the click of your mouse. With the ChemDraw 12.0 advanced drawing features, you can:

- Clean up structures
- Create synthesis drawings
- Label functional groups with nicknames.

Clean Up Structure

You may find it difficult to draw atoms in the sterically correct position. Use the Clean Up Structure command to redraw the structure so that bond lengths are fixed and atoms are in the correct location. Clean Up Structure does not position molecules relative to other objects. So, some overlap may occur.

The Clean Up Structure feature follows these rules:

- A ring is redrawn only if all of its bonds are selected.
- Structures are rotated so that as many bonds as possible are directed at a multiple of 15 degrees.
- Clean Up Structure preserves stereochemical meaning rather than the precise identity of wedged or hashed bonds, as shown below.

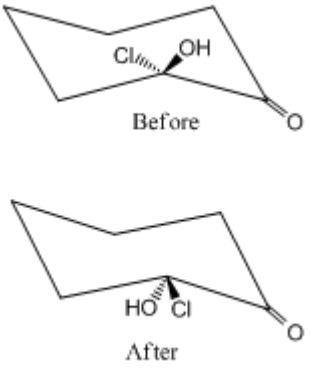


Figure 4.1 Preservation of stereochemical meaning

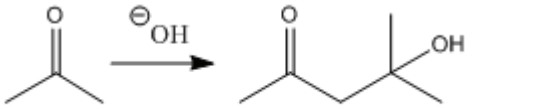
Using Clean Up Structure:

1. Select the structure or part of the structure to clean up.
2. Go to **Structure**>**Clean Up Structure** or type **Shift+Ctrl+K**.

NOTE: The Clean Up Structure command redraws your structure in iterations. Therefore, you may need to select the command more than once.

Drawing Reactions

To demonstrate how to draw reactions, we will use this example:



2-propanone 4-hydroxy-4-methylpentan-2-one

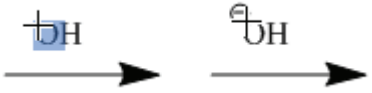
Drawing an arrow

Starting with 2-propanone, draw the reaction arrow:

1. On the Main Tool toolbar, click the Arrow tool to display the Arrow toolbar.
2. While holding the mouse button down, move the mouse to the palette title bar, then release the button. The palette becomes a floating toolbar.
3. Click the third arrow from the left in the top row.
4. In the document window, click and drag the mouse horizontally to the right of the 2-propanone structure. The arrow appears.
5. Select the Text tool.
6. Click above the arrow. A text box appears.
7. Type **OH** and press Esc. Realign the text box as necessary using a selection tool.

Add a charge symbol using the specialized symbols available in the Chemical Symbols tool palette:

1. In the Main Tool toolbar, click the Chemical Symbol tool.
2. Holding the mouse button down, select the circled **Circle Minus** symbol.
3. Point to the center of the **OH** label. Move the cursor slightly right or left to select the **O**.
4. With the oxygen atom selected, drag the charge symbol around the atom to the desired position.



Objects added from the Chemical Symbols palette are associated chemically with the structure they are near. Note that the red valence error warning disappears when you add the minus charge.

CURVED ARROWS

For some reactions, you may not want to be limited to drawing simple, straight arrows. You can curve most arrows found on the Arrows toolbar. After you paste an arrow in your drawing, click and drag the selection point in the middle of the arrow.

As you drag the selection point, the size of the arc appears, measured in degrees.

Drawing the product

We now create 4-hydroxy-4-methyl-2-pentanone using a copy of the 2-propanone structure. You can also create the product from scratch but you may find copying another structure more convenient.

Copy the structure:

1. Select the 2-propanone structure and its caption.
2. Press and hold the **Ctrl** key.

The hand pointer with a plus sign indicates that you are in the duplication mode of a selection tool.

3. Drag the selection rectangle to the right and release the mouse button.

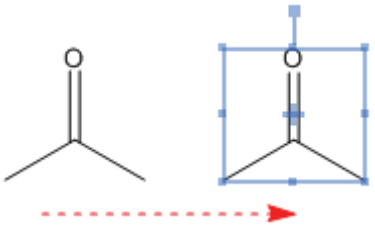


Figure 4.2 Duplicating a structure

NOTE: To keep the copy aligned with the original, hold Shift while dragging.

Modify the duplicate structure:

1. Select the Solid Bond tool.
2. Click the far right bond of the copied structure (Figure A).
3. Point to a terminal carbon, shown in A below.
4. Click the carbon atom until three bonds appear, allowing a pause between each click.

NOTE: If you click too fast, the click is interpreted either as a double-click, which opens a text box or a triple-click, which duplicates your last atom label.

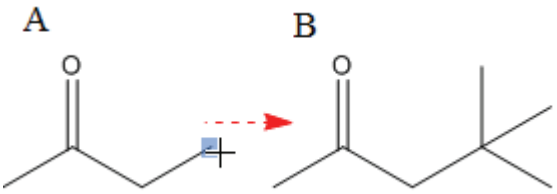


Figure 4.3 Adding multiple bonds to an atom

5. Point to a terminal carbon atom, shown in Figure A below.
6. Type **OH** in uppercase.

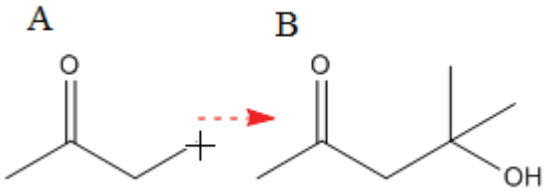


Figure 4.4 Adding an atom label

A

Chemical Interpretation

ChemDraw 12.0 converts lines, characters, and other symbols into chemically meaningful figures as you work. This occurs in the background.

This section describes how ChemDraw 12.0 interprets what you draw.

Chemical Intelligence

ChemDraw 12.0 was designed as a tool to aid in chemical communication. Most chemists would understand AcOo-C_6H_4COOH immediately, whether or not they recognized it as aspirin. Most computer programs, however, require what is known as a "complete connection table," in this case, a collection of 21 atoms connected by 5 double bonds and 16 single bonds in a specific pattern. ChemDraw 12.0 takes what makes sense to a chemist and converts it into what makes sense to another application.

This chemical intelligence can be used as a sophisticated "spelling" checker for chemical compounds. For example, if you're investigating organic acids, a compound with the structural formula CH_3COO would probably represent acetic acid. Present the same formula in a paper on transition metal chemistry, and you might be describing a novel methylated cobalt oxide. If you had asked ChemDraw 12.0 to interpret it beforehand, you would have received a message reporting a valence error, and you might have been prompted either to add a negative charge or to change the capitalization.

ChemDraw 12.0 can offer only suggestions. If you and your audience understand what you are trying to depict, then you can ignore these suggestions.

Database Conventions

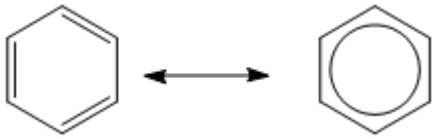
Most databases require not only that you draw a structure in a way that makes sense, but that you draw it in the way that the database expects it.

Bond Conventions

The table below describes the bond conventions ChemDraw 12.0 recognizes.

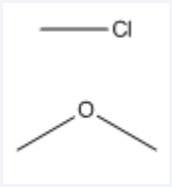
Bond	Description
	Single bond, unspecified stereochemistry.
	Single bond, "down" stereochemistry (into the plane of the paper, away from viewer); single bond, "up" stereochemistry (out of the plane of the paper, toward viewer).
	Double bond, with *cis*/*trans* stereochemistry as drawn.
	Triple bond.

A single bond near a closed circle is recognized as aromatic:

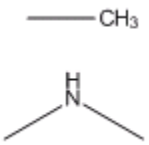


Atom Labels

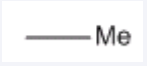
A simple atom label may contain any of the following:



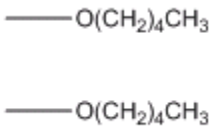
A single element.



An element and some number of hydrogen atoms.



A nickname.

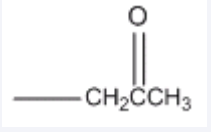


Repeating units within parentheses.

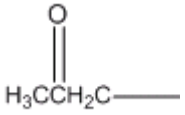
A series of any combination of the above.

ChemDraw 12.0 analyzes atom labels from left to right, applying standard valence rules to determine which atoms are bonded together. The exception is with an atom label in Automatic alignment on the left side of a compound. This type of atom label is displayed in reverse (H_3CO instead OCH_3) and is parsed from right to left. Standard valences for each atom are defined in the Isotopes Table.

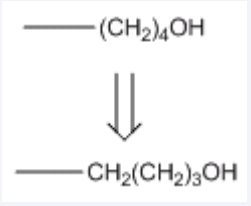
By definition, a "simple" atom label has all bonds attached to the first (or last) character. A multi-attached atom label has bonds connected to more than one character, or has all of its bonds attached to a character in the middle of the atom label. Multi-attached atom labels are always parsed from beginning to end, but the beginning might be on the right if the atom label was in Automatic style and on the left side of the original structure:



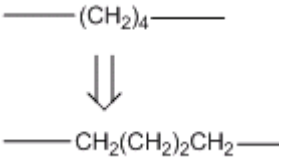
A multi-attached label that is parsed from left to right.



A multi-attached label that is parsed from right to left.

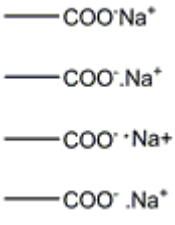
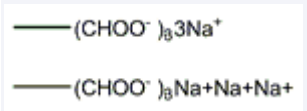


A bond attached to the open parenthesis of a repeating group is treated as if bonded to the first of those groups.



A bond attached to the close parenthesis or repeat count of a repeating group is treated as if bonded to the last of those groups.

Multiple fragments within a single label can be specified in the following ways:

	Implicitly, using standard valence rules.
	Explicitly, using a space, period (unsuperscripted or unsubscripted), bullet, or combination.
	An unsuperscripted, unsubscripted integer at the start of a fragment is recognized as a stoichiometric multiplier and is treated as if the appropriate number of fragments were drawn explicitly.

Chemically Significant Text

Often, it is simpler to write a chemical formula like MeOH or H_2O than it is to draw out an entire atoms-and-bonds structure. ChemDraw 12.0 correctly interprets any *unambiguous* structural formula. For example, $CH_3COCH_2CH_3$ is recognized as methyl ethyl ketone and MeOH is recognized as methanol. On the other hand, C_6H_6 might mean benzene one of over 200 other isomers. C_6H_6 is not recognized by ChemDraw 12.0 as a specific molecule. Generally, empirical formulas (C_2H_6 and H_2SO_4) are not recognized, but structural formulas (CH_3CH_3 and $HOSO_2OH$) are.

Chemically-significant text must be entirely in formula or, for isotopes and charges, superscript style. ChemDraw 12.0 does not recognize a chemical formula embedded within a larger block of text.

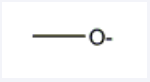
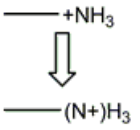
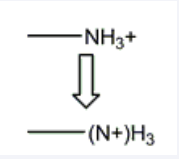
If you draw a bond, add an atom label, and then delete the bond, you have a chemically meaningful text block whose font, size, and style match other atom labels.

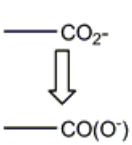
H_2O

If you create a caption with the text tool and set it to Formula style, you have a chemically meaningful text block whose font, size, and style match other captions.

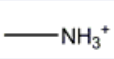
Charges

Charges may be created as part of a textual atom label or with the appropriate symbol from the Chemical Symbols palette. Charges are always assigned to a specific element in the atom label, whose acceptable valences become those of the similar isoelectronic neutral element

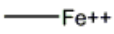
	A charge following an element is assigned to that element.
	A charge that does not follow an element is assigned to the next element.
	Charges that follow a monovalent element with a repeat count are assigned to the element before that element.



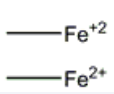
Charges that follow other repeating units are distributed among those units.



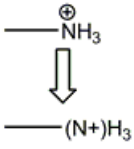
Charges may be superscripted.



Multiple charges are recognized appropriately.



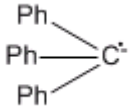
Charges may have repeat counts as long as both the charge and the repeat count are superscripted.



A “floating” charge placed with the Chemical Symbols Tool is assigned to the nearest atom. If no atom is within the distance set as the Fixed Length, the charge is ignored and not assigned to any atom.

Radicals

Radicals are indicated with the appropriate symbol from the Chemical Symbols palette. As with charges, they are assigned to the nearest atom. Radicals always occupy one free valence, in addition to any charge effects. One example is:



B

Nicknames

Nicknames are listed alphabetically by abbreviation in two tables. Each listing is a link to a page that displays the structure and full name.

A navigation bar at the bottom of the page lets you step through the section or return to the listings.

Ac-Me					
Ac	Bz	c-C7H13	cyclopropyl	DPIPS	i-C4H9
Ad	BOM	c-C8H15	Cys	DPTBS	i-C5H11
Ala	Bs	c-Hx	Dan	DTBMS	i-Pr
Alloc	Bt	C10H20	DEAE	DTBS	Ile
Allyl	Btm	C10H21	DEIPS	Et	Im
Am	Bu	Cbz	DMIPS	Fmoc	Leu
Arg	Bzh	cHx	DMPM	Gln	Lys
Asn	Bzl	CoA	DMPS	Glu	m-C6H4
Asp	BzOM	Cy	DMTr	Gly	m-Phenylene
Benzoyl	c-C3H5	cyclobutyl	DNP	His	m-Tolyl
Benzyl	c-C4H7	cycloheptyl	Dnp	i-Am	MDIPS
Bn	c-C5H9	cyclooctyl	Dns	i-Bu	MDPS
Boc	c-C6H11	cyclopentyl	DNS	i-C3H7	Me

MEM-Xyl					
MEM	n-Pr	Phenyl	s-Butyl	TBDMS	Thr
Mes	N3	Pht	s-C4H9	TBDPS	TIPDS
Met	neo-Am	Piv	s-C5H11	TBMPS	TIPS
MMTr	neo-C5H11	PMB	SEM	TBS	TMS
MOM	Np	PMBM	Ser	TDS	Tos
MPM	o-C6H4	PNB	SES	Tf	trans-Cinnamyl
Ms	o-Phenylene	Poc	t-Am	Tfa	Troc
MTM	o-Tolyl	PPi	t-BOC	TFA	Trp
n-Am	p-C6H4	Pr	t-Boc	Thexyl	Trt
n-Bu	p-Phenylene	Pro	t-Bu	THF	Ts
n-C3H7	p-Tolyl	Pv	t-Butyl	Thf	Tyr
n-C4H9	Ph	s-Am	t-C4H9	THP	Val
n-C5H11	Phe	s-Bu	t-C5H11	Thp	Xyl

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