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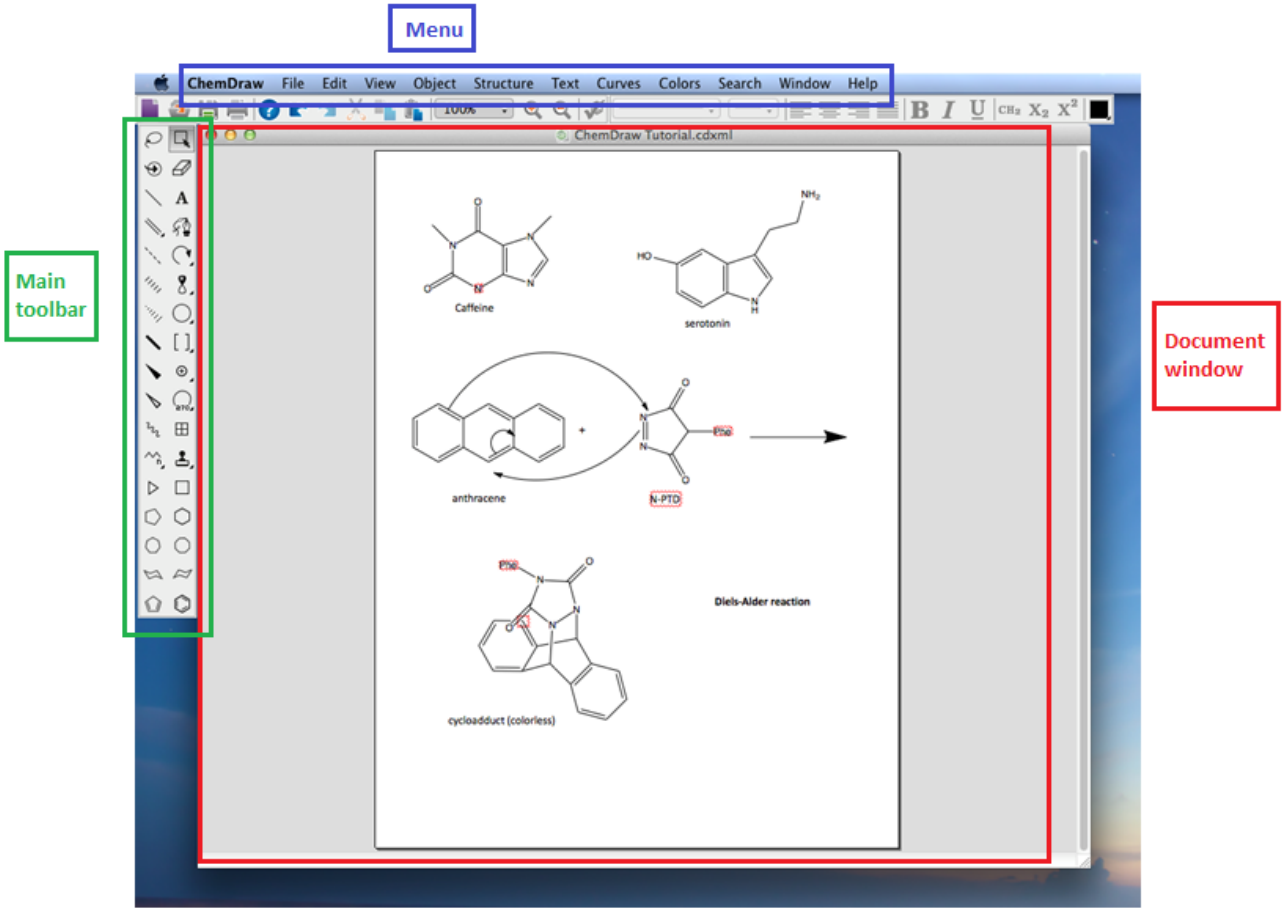
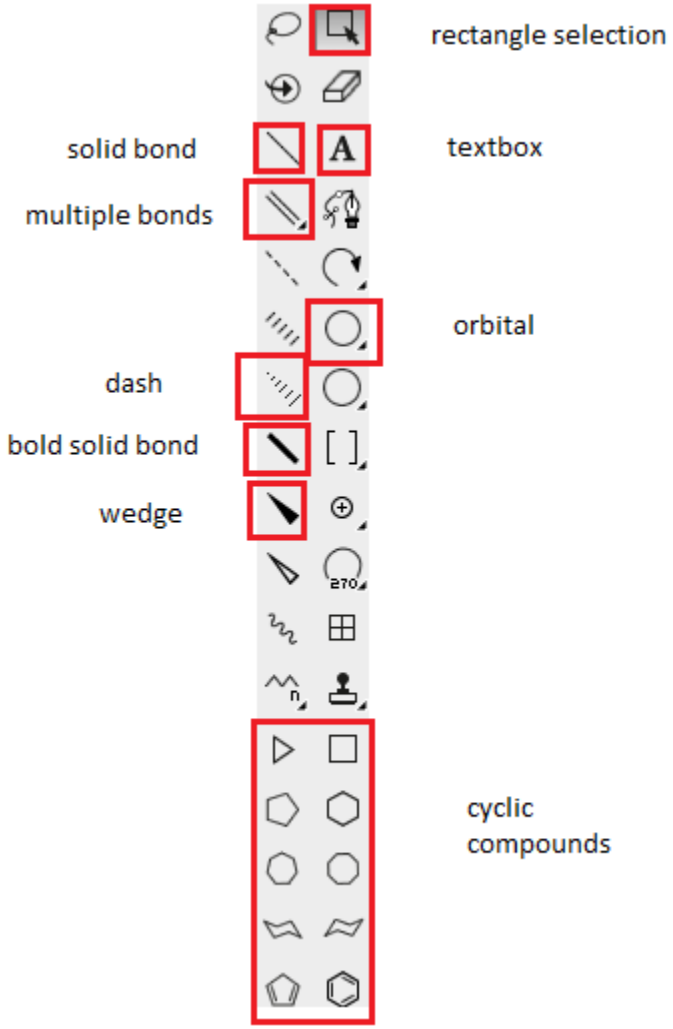
Introduction to ChemDraw

Adapted from Cambridgesoft Online Tutorial
http://www.cambridgesoft.com/support/DesktopSupport/documentation/manuals/files/chembiodraw.pdf

1. Elements in ChemDraw





2. Bonds

To draw a bond, choose the solid bond tool from the Main toolbar on the left.

Fixed bond length - Fixed bond angle

- Object>Fixed Lengths and/or **Fixed Angles** and if a check mark is next to the **Fixed length** and/ or **Fixed Angles** command, the bond in the structure will be of a default length and/or bond angle. The default setting helps keep the angles and bond lengths appropriate for the structure. The default bond length is .4167 inch and bond angle is 120° (relative to the X-axis)

- Uncheck the **Fixed length** and/or **Fixed Angles** command to draw any bond lengths and angles.

Changing fixed bond length - bond angle

File>Document Settings>Drawing and enter values in the **Fixed Length** and/or **Chain Angle** textbox **> OK**

Double bonds/ Partial Double Bonds/ Triple Bonds

Choose the desired type of bonds from the **Multiple Bonds** box on the Main toolbar

Bond crossing

Indicating which bond in the front by

1. Select the bond that should be in the front
2. Go to **Object>Bring to front**

or alternatively,

1. Select the bond that should be at the back
2. Go to **Object>Send to back**

3. Atom labels

Annotate atoms/groups

Choose the **Text** tool from Main toolbar, click on the position of the atoms/groups on the structure and start typing.

Edit the annotation
Choose the **Text** tool again and click on the text on the structure.

Format text color, font, size and style
1. Select text object with the selection tool from the Main toolbar
2. Go to **Object>Object settings>Atom Labels** and modify the settings **>OK**

Show/Hide label on terminal Carbons and/or implicit Hydrogen
Go to **File>Document settings>Atom labels** and check/uncheck **Show labels on Teminal Carbons** and/or **Hide Implicit Hydrogens** boxes at the bottom of the window **>OK**

4. Rings

To draw a cyclic compound, choose the **Ring** tool from the Main toolbar. Hold the mouse while dragging the to orient the ring.
If you click on an atom or bond with a ring tool selected, the ring will be fused to the atom or bond.

Delocalized rings
To draw a delocalized ring, choose a **Ring** tool, hold Command on the keyboard while clicking on the document window.

Reducing ring size
For example, if you want to convert cyclohexane to cyclopentane, choose a bond tool, point at an atom while holding Shift and start dragging the atom onto the next one. The bond between the two atoms will disappear.

5. Moving/Rotating Objects

Moving an object
Select the object with the **Rectangle Selection** tool from the Main toolbar, click and drag the object to a new location

Rotating an object
Select the object with the **Rectangle Selection** tool from the Main toolbar. The Rotation handle is at the top of the selection area. Rotate the structure while clicking on the Rotation handle.

Rotating an object by a specific angle
1. Select the object with the Rectangle Selection tool from the Main toolbar.
2. Go to **Object>Rotate** and enter the desired angle for rotation

6. Newman Projection

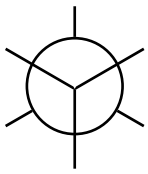


Figure 6

For example, to draw a Newman Projection of ethane (**Figure 6**)

1. Choose the **Solid bond** tool from the Main toolbar. Draw a strcture as shown in **Figure 6.1**
2. Choose an **s Orbital** from the **Orbital** tool on the Main toolbar. Click on the tertiary carbon atom in the front to insert a circle.
3. Choose the **Selection** tool from the Main toolbar, click on the three bonds of the tertiary carbon atom at the back while holding the Shift key to choose all the bonds (**Figure 6.2**). Go to Object>Bring to front.
4. Drag the selected parts until the carbon is centered in the orbital.

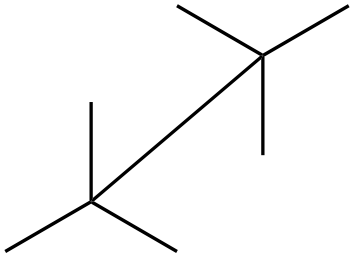


Figure 6.1

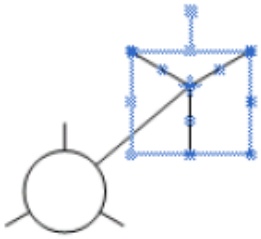


Figure 6.2

7. Perspective Drawing

For example, to draw α-D-glucose (**Figure 7**)

1. Choose Cyclohexane tool from the Main toolbar. Choose the selection tool from the Main toolbar to select the structure. Drag the structure to the right until it is about 200% stretched
2. Add bonds and label atoms
3. To enhance the front bond: choose the **Bold bond** tool from the Main toolbar and click on the front bond
4. To enhance the side bonds, choose the **Wedge bond** too from the Main toolbar and click on the two side bonds.

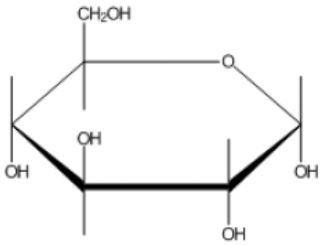


Figure 7

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