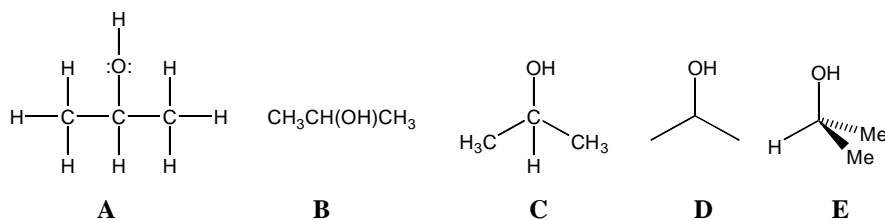


1. An Introduction to ChemDraw

Introduction

ChemDraw can be used to draw simple two-dimensional representations of organic molecules. These structures must precisely describe the connectivity of atoms. Five different representations of 2-propanol (isopropanol or "rubbing alcohol") are shown below. While structure **A** shows all bonds and lone pairs of electrons, a number of short-cuts are often used when drawing molecules. For example, $-\text{CH}_3$ is used to represent the methyl groups in (**B**) and (**C**).



Bond-line structures (**D**) are often the simplest representation of organic molecules. A chain of carbon atoms is shown as a series of lines; each angle between lines and each line end is a carbon atom. The carbon atoms are not labeled. All heteroatoms (*i.e.*, N, O, S, halogens) are labeled. Hydrogens on carbons are not shown, although it is assumed that they are present to account for the tetravalency of carbon. Since sp^3 carbon atoms are tetrahedral it is often useful to show the structure of organic molecules using wedge-and-dash structures (**E**). The wedge indicates a bond coming out of the page toward you, the dashed bond is going into the page. In structure **E** the methyl groups are abbreviated as "Me". Other common abbreviations for substituents are Et (ethyl), *i*-Pr (isopropyl), *t*-Bu (*tert*-butyl). ChemDraw can also be used to draw Newman and Fischer projections of organic molecules (see your textbook).




Getting Started

The ChemDraw screen has a vertical palette of *tools* on the left, a series of pull-down *menus* at the top of the screen, and a blank window on which to draw.

The following instructions illustrate how to draw molecules. Work through the step-by-step instructions to draw the structure of 2-propanol shown on the right.

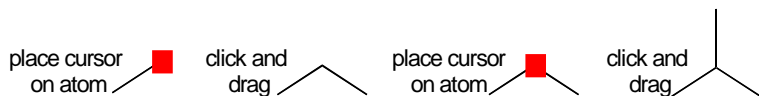


- i. Launch ChemDraw by clicking on the program icon (or use the start menu).
- ii. First you will draw a bond: Click on the bond drawing tool in the palette on the left-hand side of the screen. Move the cursor to the blank window, click-hold-drag-and-release the mouse to draw a bond.

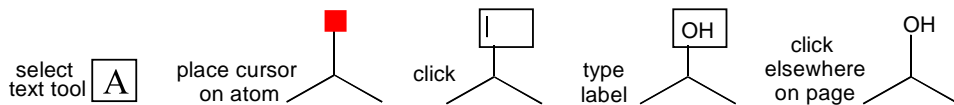
select bond drawing tool  place cursor on page + click  drag 

Each end of the bond represents a carbon atom until you change it to another type of atom (see below).

- iii. You will now draw the other bonds: Place the cursor on one end of the bond; a black square will appear. Click-and-drag the mouse to draw a second bond. Click-and-drag from the middle atom to draw a third bond.

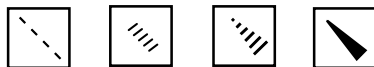


- iv. One of the carbon atoms should be changed to a hydroxyl group: Click on the text tool; place the cursor on the atom you want to label, a black square will appear. Click the mouse when the end of a bond is highlighted with a black square, a text box will appear. Type OH using the keyboard, and then click the mouse elsewhere on the window. Numbers entered in atom labels are automatically written as subscripts.



Other Drawing Tools

A series of bond drawing tools are available to show the three-dimensional arrangement of atoms.

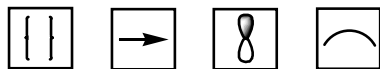


Double bonds are made by clicking on an atom and dragging along an existing bond to an adjacent atom. A number of ring structures can be drawn automatically. Work through the following example.

- i. Select the five-membered ring tool, click-and-drag on the drawing window and see what happens.
- ii. Now select the bond drawing tool, click on an atom in the five membered ring (the structure of cyclopentane), drag to an adjacent atom and release. A double bond will appear (to give the structure of cyclopentene).



Other tools allow you to draw brackets, arrows, orbitals and curves. To use these, click-and-hold on the tool palette, move the mouse to select the particular type of object you want, *then* release. Then click-and-drag on the drawing window.



Moving and Rotating Structures

Draw a molecule and then move, shrink or enlarge, and rotate it using the following instructions.

- i. *Click on the Lasso tool. Click on the window close to a molecule you want to move; hold down the mouse, circle around the molecule and release. The circled molecule will be highlighted in a highlight box.*
- ii. *To move the molecule: Move the cursor into the middle of the box until a hand appears. Click-and-drag to move the highlighted molecule.*
- iii. *To shrink or enlarge the molecule: Move the cursor to the bottom right corner of the highlight box (a double-headed arrow will appear). Click-and-drag to shrink and enlarge the highlighted molecule.*
- iv. *To rotate the molecule: Put the cursor at the top right corner of the highlight box (a curved arrow will appear). Click and drag to rotate the highlighted molecule.*



Text can be written anywhere on the window by choosing the Text tool and clicking on the drawing window (NOT on an atom). Font, size and style (*i.e.*, italics, underlining) can be changed using the Text menu. The Object menu lets you further manipulate highlighted items. ChemDraw can be used to prepare structures, reaction schemes and mechanisms as answers to homework questions from your textbook, and to illustrate lab reports.