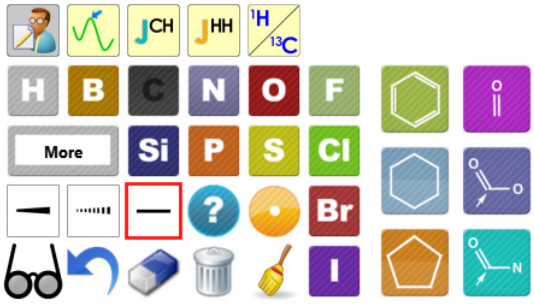
Chapter 4
Sketching Organic Molecules in 2D

The tutorials in this chapter introduce and illustrate tools to sketch organic molecules in 2D and then to convert them into realistic 3D structures.

Not only are 2D sketches ("drawings") more familiar to most chemists than 3D structures, they are typically easier to produce especially for complex molecules that may incorporate fused rings or require stereochemistry to be defined. The advent of touch-screen computers makes the argument for sketching as an alternative to building even more compelling. Molecules that require several minutes to build in 3D can be drawn in seconds. The key is automatic and reliable conversion from 2D drawings to 3D structures and from 3D structures to 2D drawings.

Sketch Palette

The sketch palette contains tools for making and manipulating 2D drawings, including tools for adding cues to designate stereochemistry.*



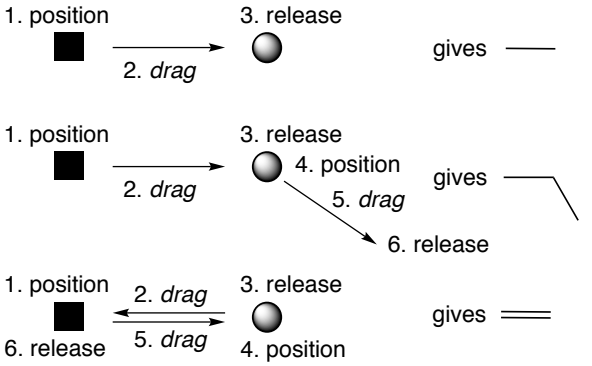
These include atoms that are most commonly found in organic molecules (H, B, C, N, O, F, Si, P, S, Cl, Br and I), the phenyl,

* A row of icons appears immediately above the sketch palette. These are intended to add arrows to designate reaction transition states and to append experimental NMR chemical shifts and observed HH and CH couplings to the sketch palette

cyclohexyl and cyclopentyl rings and the carbonyl, acid/ester and amide functional groups. The button immediately below H and B atoms allows for entering additional elements, functional groups, and ligands. The palette also contains stereochemical markers and charge/radical markers. Complete details are found in **Chapter 20**.

Sketching a Molecule

To start a sketch, first select (*click* on) an atom, group, ring or wildcard icon in the palette and then *double click* in the white portion of the screen (the drawing area). To draw a bond, first *click* on an atom, group, ring or wildcard icon in the palette to designate what is at the end of the bond, then position the cursor over the atom in the drawing area where you want the bond to start, move the cursor while holding down the left button ("*drag*" the cursor) to the place in the drawing area where you want the bond to end and release the button. Multiple bonds are made by dragging over existing bonds.*



To make a bond touch the screen where you want it to start, move one finger to where you want it to end and lift. Replace position by touch, drag by move and release by lift in the diagram above.

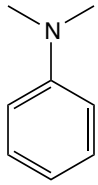
* With ***Spartan'20***, and alternative way of drawing multiple bonds is simply to *double click* on a single bond. *Double clicking* (on a double bond) draws a triple bond and *double clicking* on a triple bond reverts to a single bond. The one exception is *double clicking* on a bond when a ring is selected in the palette as this signifies ring fusing.

Manipulating a Sketch

To translate the sketch, move the mouse over the screen while holding down the right button. To rotate the sketch (in the plane of the screen), move the mouse up and down while holding down both the left button and **Shift** key. Use the scroll wheel to resize the sketch.

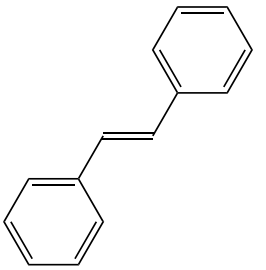
To translate the sketch, move two fingers over the screen. To rotate the sketch in the plane of the screen, "twist" two fingers on the screen. To resize the sketch, pinch (or spread) two fingers on the screen.

N,N-Dimethylaniline

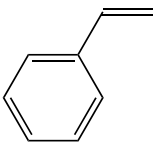


1. Select **New Sketch** from the **File** menu (or *click* on at the top of the screen) to bring up the sketch pad. *Click* on ( ) in the palette and *double click* on screen.
2. *Click* on (N) in the palette. Position the cursor over the "top" carbon on the benzene ring, *drag* it up and release. You have drawn aniline.
3. *Click* on (C) in the palette. Position the cursor over the nitrogen, *drag* it up and to the left and release. (C) is still selected. Again position the cursor over the nitrogen, *drag* it up and to the right and release.
4. *Click* on ( ) in the palette to clean up your drawing and *click* on ( ) to produce a 3D structure. The name ***N,N-dimethylaniline*** will appear at the bottom of the screen as the molecule is in SSPD.
5. Close ***N,N-dimethylaniline***.

***trans*-Stilbene**

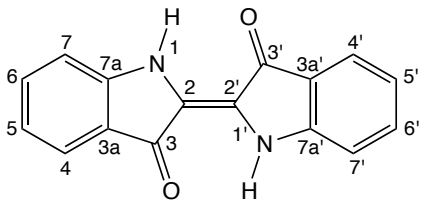


1. Select **New Sketch** from the **File** menu ( ) to bring up the sketch pad. *Click* on (C) in the palette. Position the cursor on the screen, *drag* it to the right and release. Position the cursor on one end of the line (CC bond) that you have just drawn, *drag* it to the other end and release. You have drawn ethylene.
2. *Click* on ( ). Position the cursor over the left end of the double bond, *drag* it down and to the left and release. You have drawn styrene.



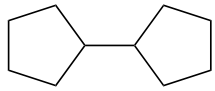
3. ( ) is still selected. Position the cursor over the right end of the double bond, *drag* it up and to the right and release. You are done.
4. *Click* on ( ) to clean up your drawing. *Click* on ( ) to convert it to a 3D structure. The name ***trans-stilbene*** will appear at the bottom of the screen as the molecule is in SSPD.
5. Close ***trans-stilbene***.

Indigo

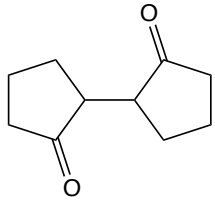


1. Select **New Sketch** from the **File** menu ( ). *Click* on ( ) and *double click* on screen.

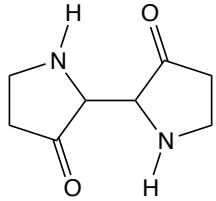
2. ( ) is still selected. Position the cursor over C_2 (see numbering in diagram above), *drag* it to the right and release. Your sketch should appear as below.



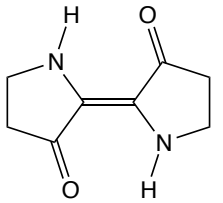
3. Select (O) from the palette. Position the cursor above C_3, *drag* it away from the ring and release. Again position the cursor above C_3, drag it along the CO bond to the oxygen and release. Alternatively, *double click* on the CO bond that you have just made to turn it into a double bond. Repeat for C_3'. You are left with a drawing.



4. Select (N) from the palette and one after another *double click* on C_1 and C_1'.



5. Select (C) from the palette. Position the cursor above C_2, *drag* it to C_2' and release. Alternatively, *double click* on the C_2-C_2' bond.

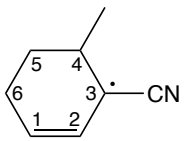


6. Select ( ) from the palette and *double click* on the bond connecting C_{3a} and C_{7a}.* Repeat for $C_{3a'}$ and $C_{7a'}$.

7. *Click* on ( ) to clean up your drawing and *click* on ( ) to turn it into a 3D structure. The name ***indigo*** will appear at the bottom of the screen as the molecule is in SSPD.

8. Close ***indigo***.

3-Cyano-4-methylcyclohexenyl Radical



This tutorial shows you how to use a wildcard to specify a functional group and how to designate a radical site.

1. Select **New Sketch** from the **File** menu ( ). *Click* on ( ) in the palette and *double click* on screen.

2. *Click* on (C) in the palette. Position the cursor over C_4 (see diagram above for numbering), *drag* it up and to the right and release. You have drawn methylcyclohexane.

3. (C) is still selected. Position the cursor over C_1, *drag* to C_2 and release. Alternatively *double click* on the C_1-C_2 bond. You have drawn 4-methylcyclohexene.

4. *Double-click* on the wildcard icon that is located immediately below H and B in the palette. *Click* on the **Groups** tab and *click* on **CN**. **CN** now appears as the wildcard icon. Position the cursor over C_3, and *drag* it away from the ring and release. You have drawn 3-cyano-4-methylcyclohexene.

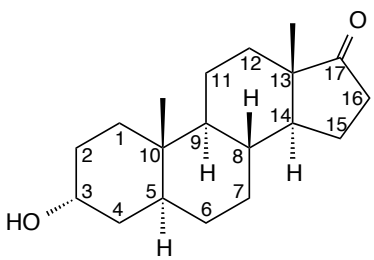
* This is the exception referred to earlier regarding *double clicking* on a bond to change it from single to double (or double to triple).

5. One of these icons () will appear in the palette directly below (). If it is not (), *click* on the icon until the icon is (). *Double click* on C_3. A "dot" (radical marker) will appear next to C_3.

6. *Click* on () to clean up your drawing and *click* on () to make a 3D structure.

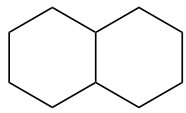
7. Close ***3-cyano-4-methylcyclohexenyl radical***.

Androsterone

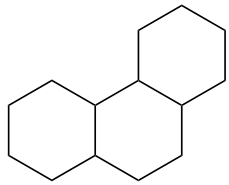


The steroid androsterone is typical example of a molecule that is difficult to build (3D) but quite easy to sketch (2D).

1. Select **New Sketch** from the **File** menu () to bring up the sketch pad. *Click* on () and *double click* on screen. Cyclohexane is still selected. *Double click* on the C_5-C_{10} bond (see diagram above).



2. Cyclohexane is still selected. *Double click* on the C_8-C_9 bond.



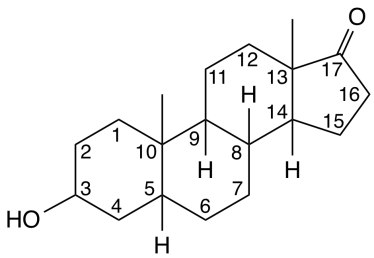
3. *Click* on () and *double click* on the C_{13}-C_{14} bond. You have now drawn the complete steroid skeleton.

4. It is necessary to explicitly specify hydrogens at C_5, C_8, C_9 and C_{14} in order to incorporate the necessary stereochemical cues (up and down "wedges") in your drawing. *Click* on (H), position the cursor over C_5, *drag* away from the ring and release. Repeat for C_8, C_9 and C_{14}.

5. *Click* on (C), position the cursor over C_{10}, *drag* up and release. Repeat for C_{13}.

6. *Click* on (O). Position the cursor over C_3, *drag* down and to the left and release.

7. (O) is still selected. Position the cursor over C_{17}, *drag* up and to the right and release. Convert the single (CO) bond at C_{17} to a double bond. Again position the cursor over C_{17}, *drag* along the bond to oxygen and release. Alternatively, *double click* on the CO single bond to turn it into a double bond. Your structure should now look as follows.



8. *Click* on (—). Position the cursor over C_{10}, *drag* along the bond to the methyl group that you drew in step 5 and release. Repeat for C_{13}. Position the cursor over C_8, *drag* along the CH bond that you drew in step 4 and release. Up wedges will appear for all three centers.

9. *Click* on (—). Position the cursor over C_3, *drag* along the CO bond that you made in step 6 and release. Position the cursor over C_5, *drag* along the CH bond that you made in step 4 and release. Repeat for the CH bonds at C_9 and C_{14}. Down wedges will appear for all four centers.

Spartan'20 offers an alternative way to specify stereochemistry. Replace steps 4-6 and 8-9 by steps A-D.

A. *Click* on ( ) in the sketch palette. *Click* on (H) (( ) remains selected), position the cursor over C_8, *drag* up and release.

B. *Click* on ( ). (H) remains selected. One after the other, position the cursor over C_5, C_8, and C_{14}, *drag* down and release.

C. *Click* on ( ) and then on (C). One after the other, position the cursor over C_{10}, and C_{13}, *drag* down and release.

D. *Click* on ( ) and then on (O). Position the cursor over C_3, *drag* down and to the left and release.

10. *Click* on ( ) to clean up your drawing. *Click* on ( ). The name ***androsterone*** should appear at the bottom right of the screen as the molecule is in SSPD. If it does not, you have made an error somewhere. Select **Edit Sketch** from the **Build** menu or *click* on ( ) if it appears at the top of the screen to return to the sketch pad.

11. Androsterone incorporates seven chiral centers. To view the R/S assignment, *click* on the **R/S Chirality** entry in the **Model** menu (R/S). R/S labels will appear next to each of the chiral centers.

12. Close ***androsterone***.