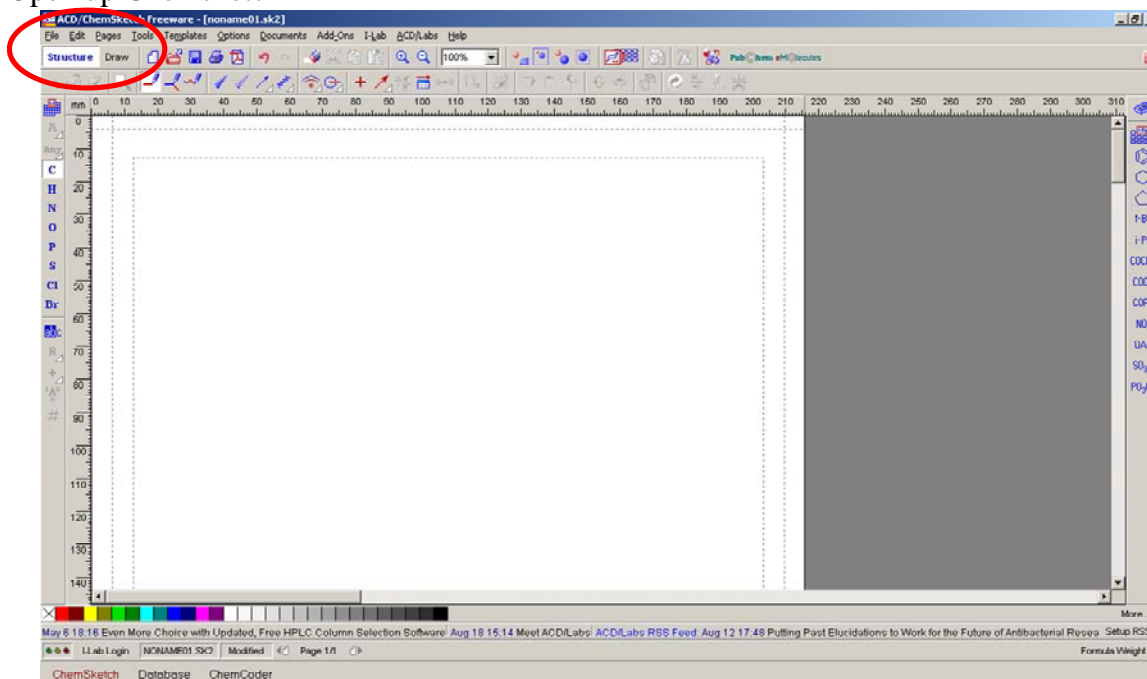


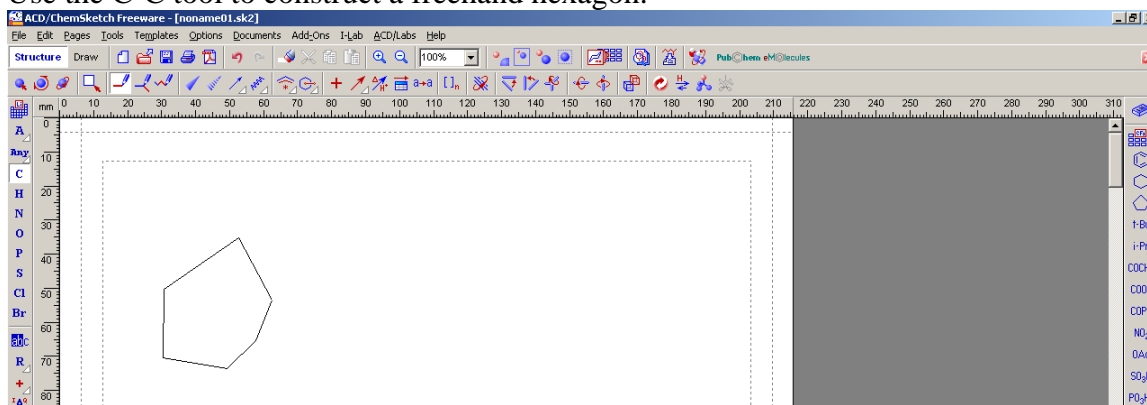
## Open up Chemsketch



There are two screens "Structure" and "Draw."

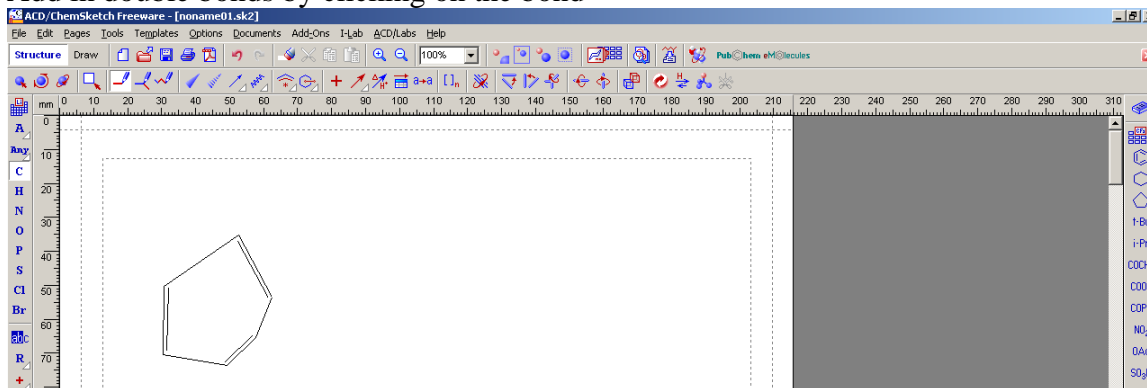
We are going to focus on the "Structure" screen since this is where molecules are constructed.

Use the C-C tool to construct a freehand hexagon.



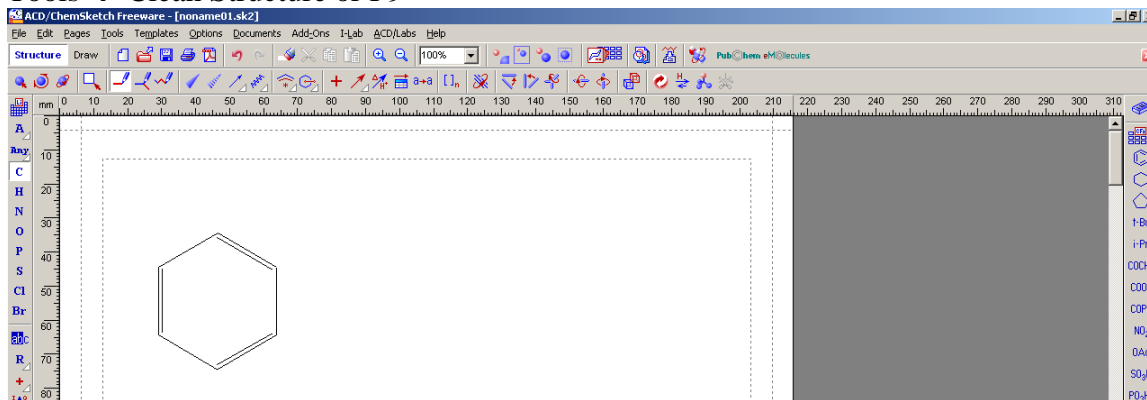
It doesn't even have to be a good hexagon!

Add in double bonds by clicking on the bond



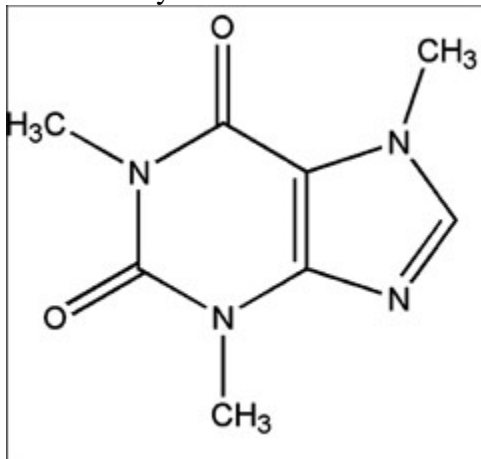
Clean it up!

Tools → Clean Structure or F9



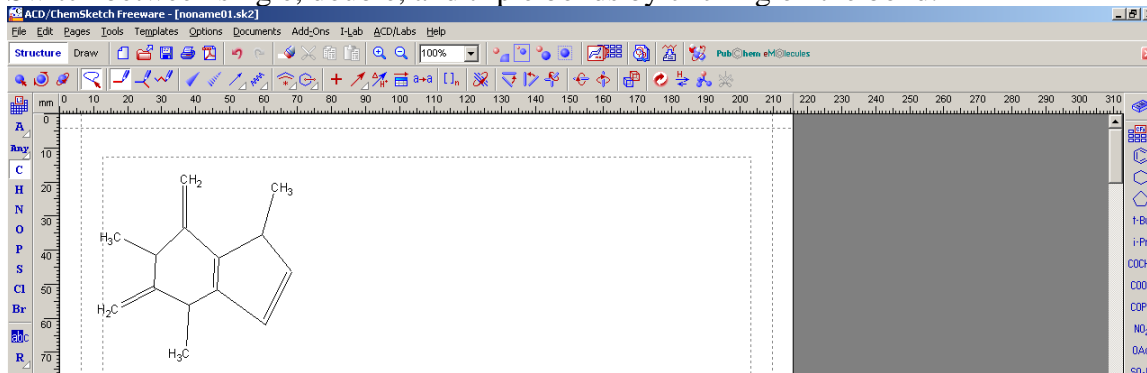
Yes!

Let's modify our benzene into caffeine

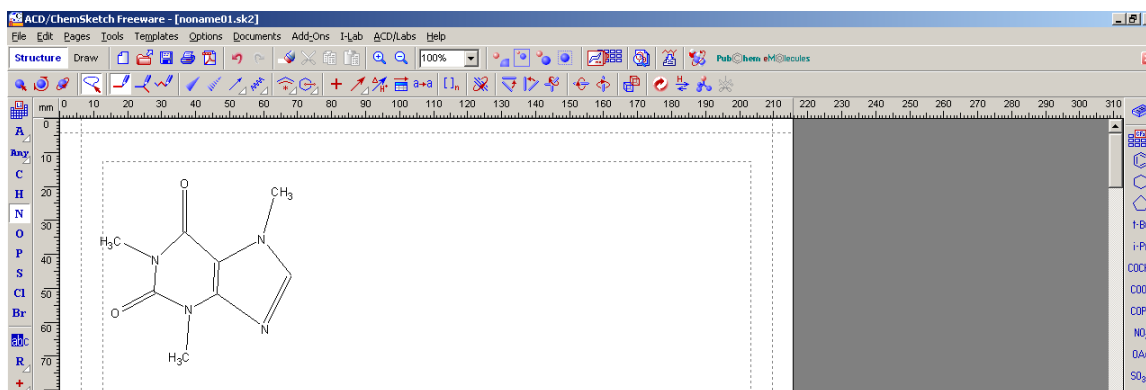


First put in all the necessary bonds.

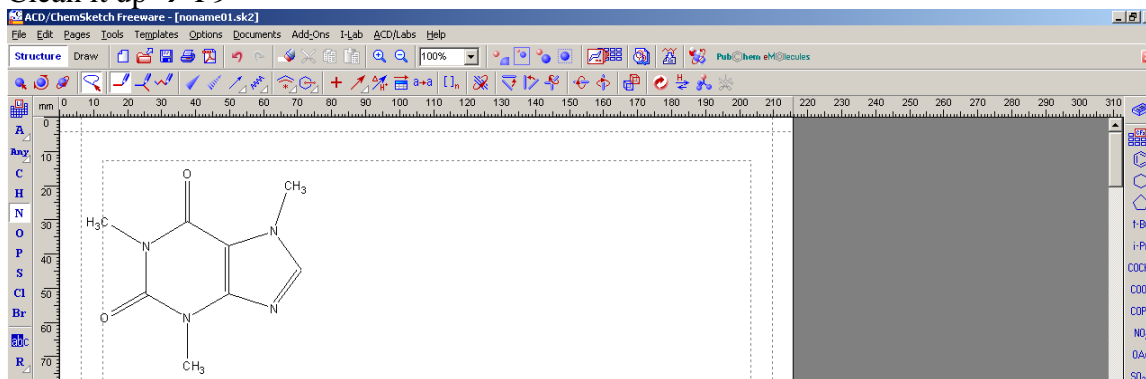
Switch between single, double, and triple bonds by clicking on the bond.



Put in the atoms → choose the atoms from the left menu.



Clean it up → F9



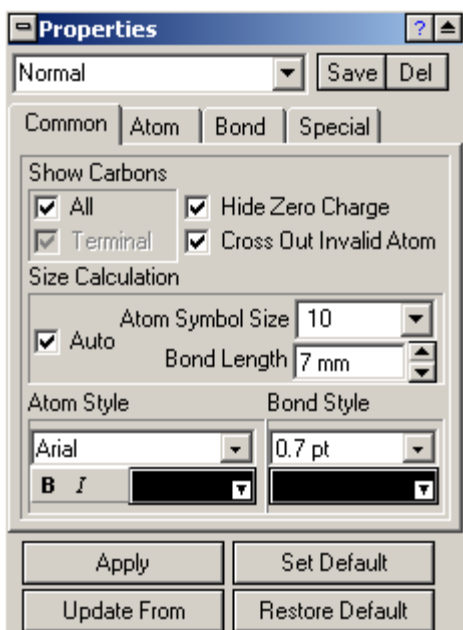
Put in the “hidden” carbons and hydrogens

I had go into Tools → Structure Properties (Alt+Shift+S)

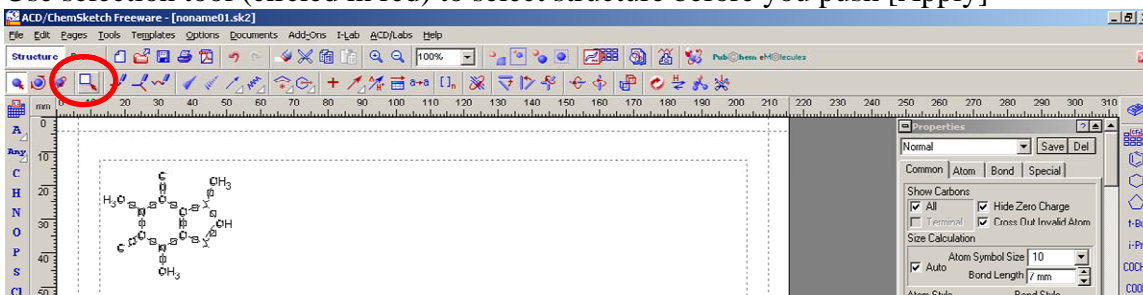
The screenshot shows the ACD/ChemSketch Freeware interface with the Properties dialog box open. The dialog box has several tabs: Normal, Atom, Bond, and Special. The 'Show Carbons' section is checked, and the 'All' checkbox is also checked. The 'Terminal' checkbox is checked, and the 'Cross Out Invalid Atom' checkbox is checked. The 'Size Calculation' section has 'Atom Symbol Size' set to 10 and 'Bond Length' set to 7 mm. The 'Atom Style' section has 'Atom Style' set to Arial and 'Bond Style' set to 0.7 pt. The 'Apply' button is highlighted. The main canvas shows the chemical structure of caffeine with all carbon and hydrogen atoms visible. The structure is a fused bicyclic system consisting of a pyrimidine ring fused to an imidazole ring. The pyrimidine ring has two carbonyl groups and two methyl groups attached to its nitrogen atoms. The imidazole ring has one methyl group attached to its nitrogen atom.

Check “All” under show carbons

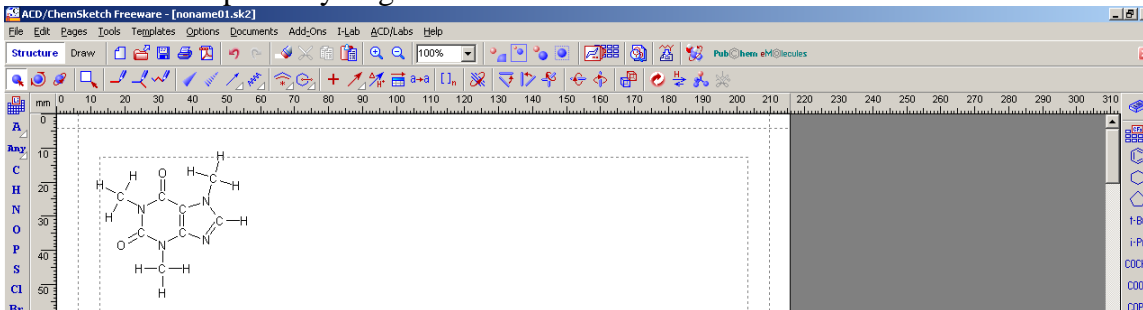
Select structure with selection tool.



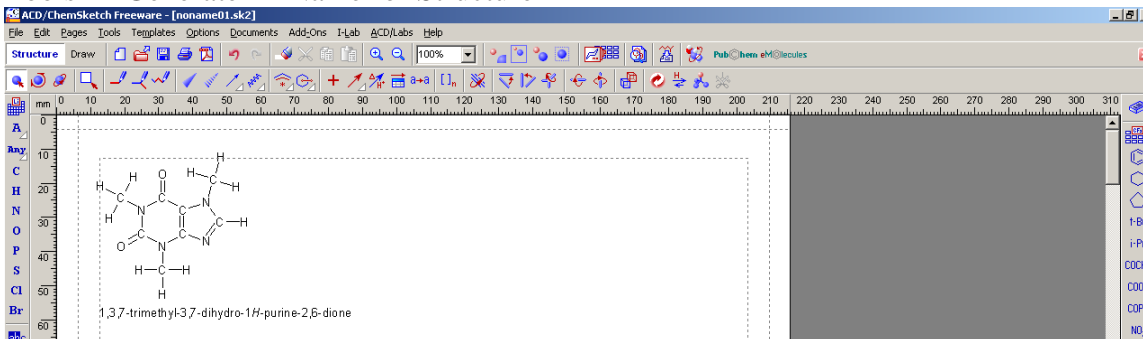
Use selection tool (circled in red) to select structure before you push [Apply]



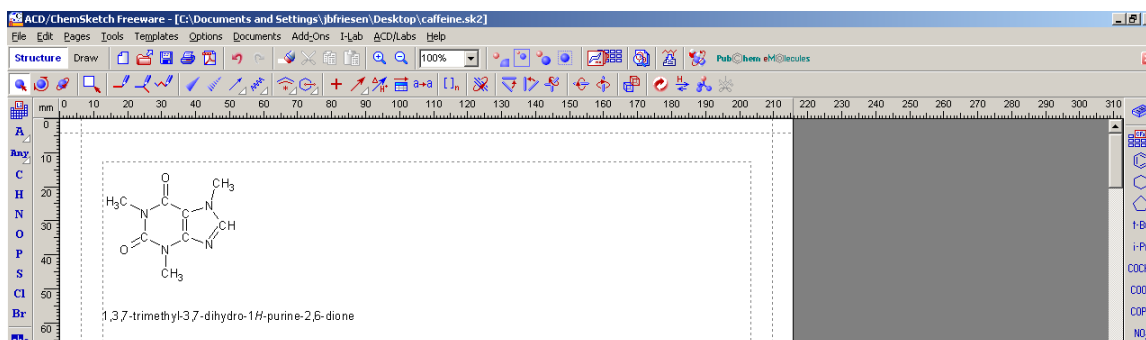
Tools → Add Explicit Hydrogens



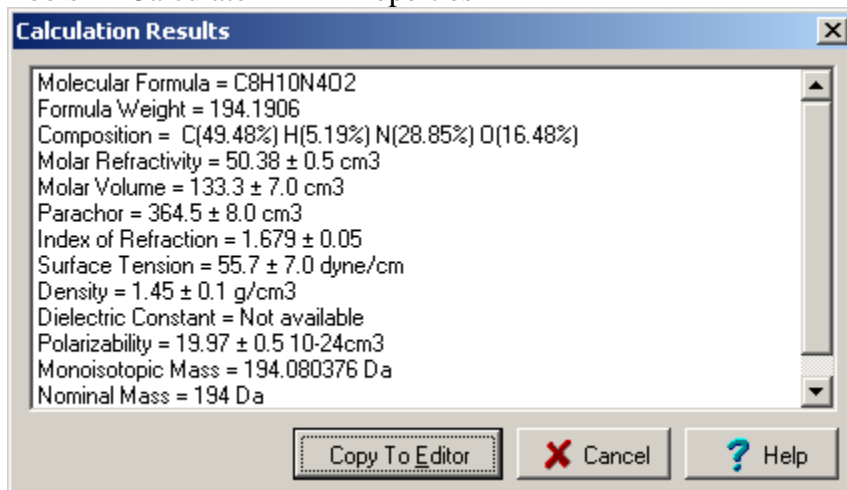
Tools → Generate → Name for Structure



Tools → Remove Explicit Hydrogens



Tools → Calculate → All Properties

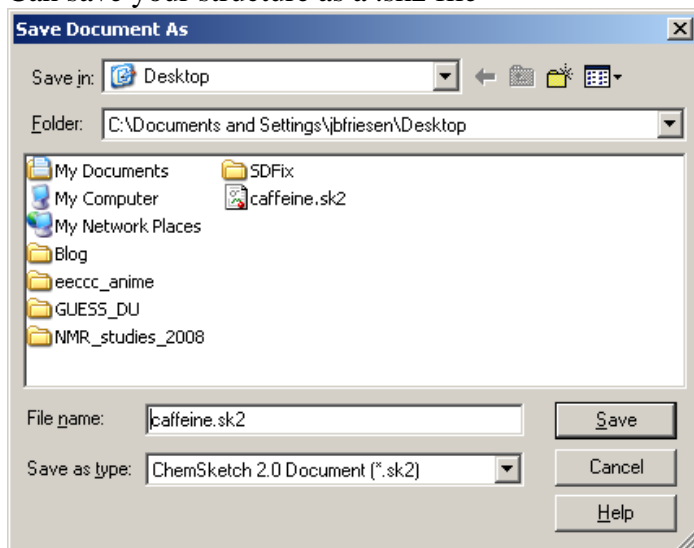


**Calculation Results**

Molecular Formula = C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>  
Formula Weight = 194.1906  
Composition = C(49.48%) H(5.19%) N(28.85%) O(16.48%)  
Molar Refractivity = 50.38 ± 0.5 cm<sup>3</sup>  
Molar Volume = 133.3 ± 7.0 cm<sup>3</sup>  
Parachor = 364.5 ± 8.0 cm<sup>3</sup>  
Index of Refraction = 1.679 ± 0.05  
Surface Tension = 55.7 ± 7.0 dyne/cm  
Density = 1.45 ± 0.1 g/cm<sup>3</sup>  
Dielectric Constant = Not available  
Polarizability = 19.97 ± 0.5 10<sup>-24</sup>cm<sup>3</sup>  
Monoisotopic Mass = 194.080376 Da  
Nominal Mass = 194 Da

Copy To Editor    Cancel    Help

Can save your structure as a .sk2 file



**Save Document As**

Save in: Desktop

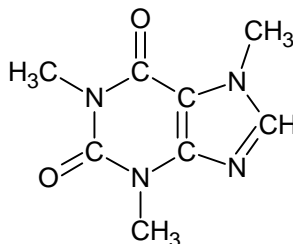
Folder: C:\Documents and Settings\jbfriesen\Desktop

File name: caffeine.sk2

Save as type: ChemSketch 2.0 Document (\*.sk2)

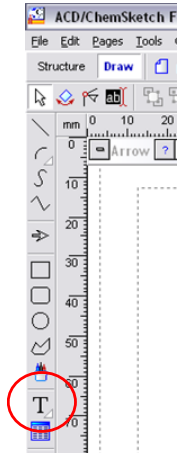
Save    Cancel    Help

And/Or you can select the structure and copy [Ctrl+C] to paste it into a word document [Ctrl+V].



How to put in unshared pairs?

In the “Draw” screen, go to the “Text” icon



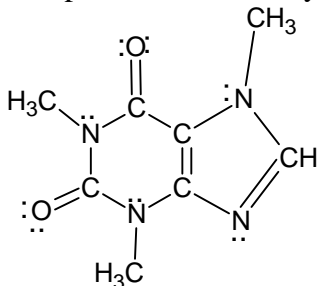
Then make two periods → .. or a colon → : and use them as your unshared pairs.

Highlight them and make them bold ([Ctrl]+[B])

You can move them around by pointing at them and dragging.

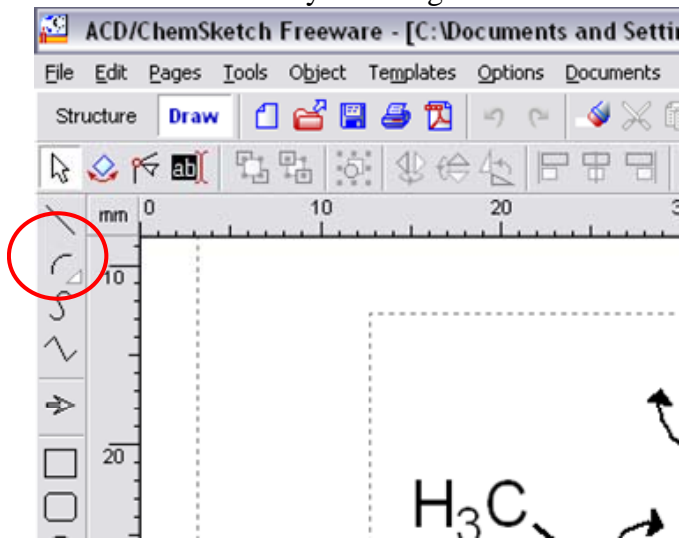
Holding down [Ctrl] as you drag allows you to copy them.

The problem is that they disappear as you drag them!

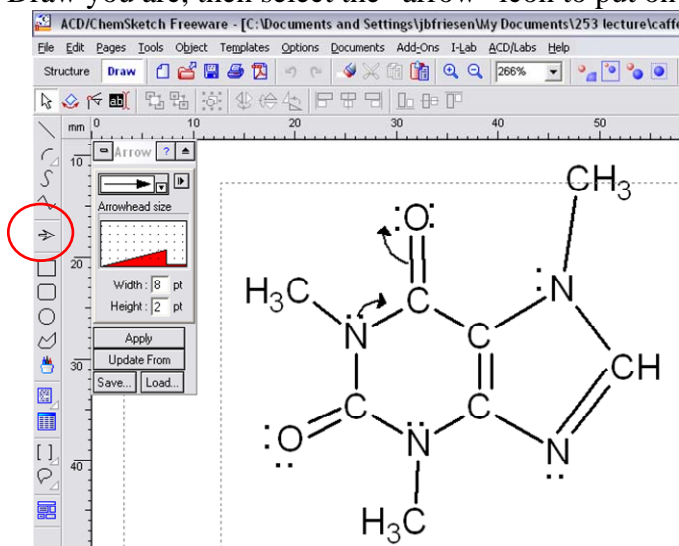


Draw some resonance structures of caffeine.

You can draw arrows by selecting the “arc” icon in “Draw” mode.

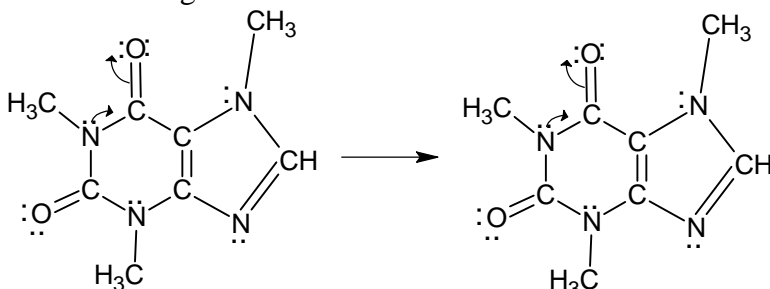


Draw you arc, then select the “arrow” icon to put on an arrow.

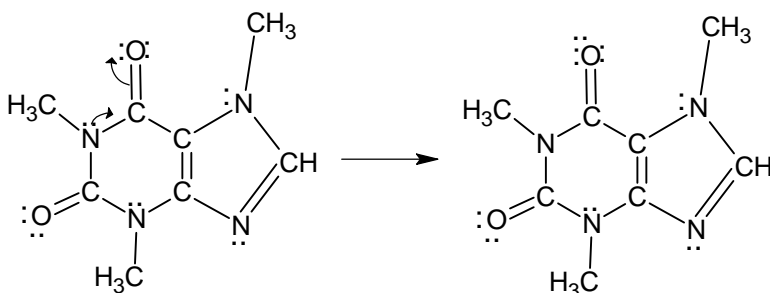


Copy your caffeine molecule, Edit → Select All, [Ctrl] to copy and drag.

Add in a straight arrow.

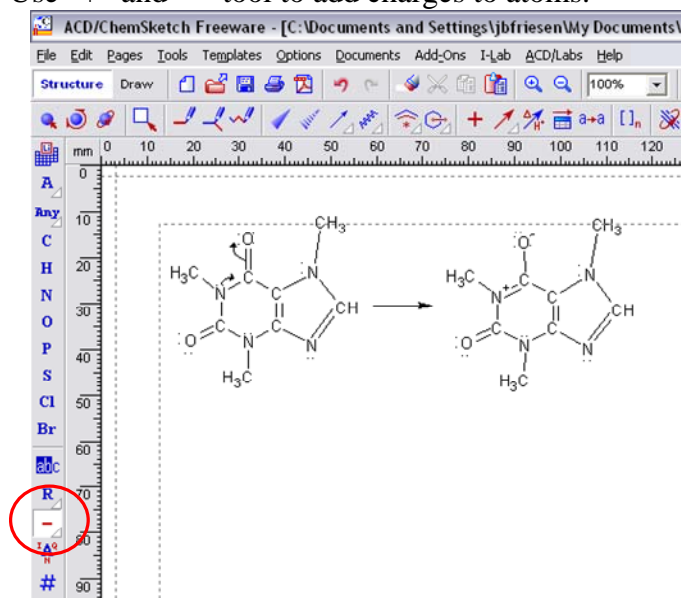


Delete the curved arrow on the right structure and move the electrons from N to O.



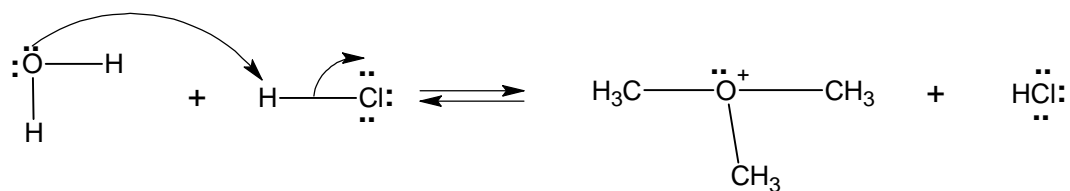
In “Structure” screen click on the “C” icon to get back to structure drawing tool to change order of bonds (single/double)

Use “+” and “-“ tool to add charges to atoms.



Want more practice with unshared pairs and arrows?

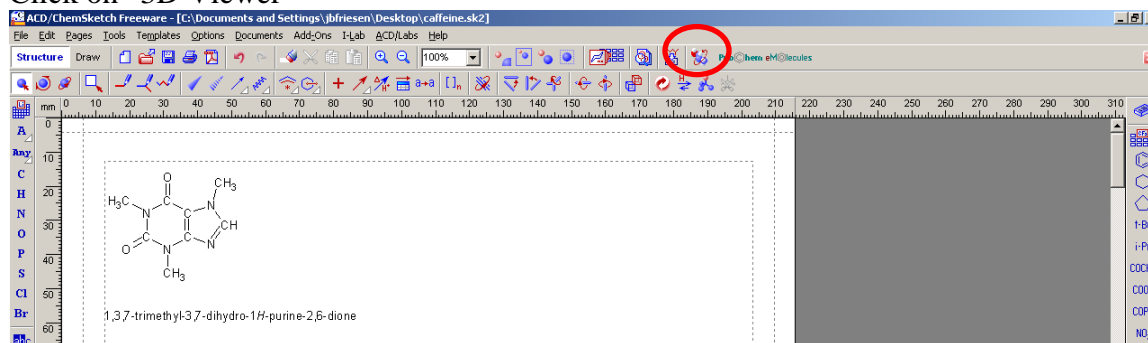
Try a simple acid-base reaction.



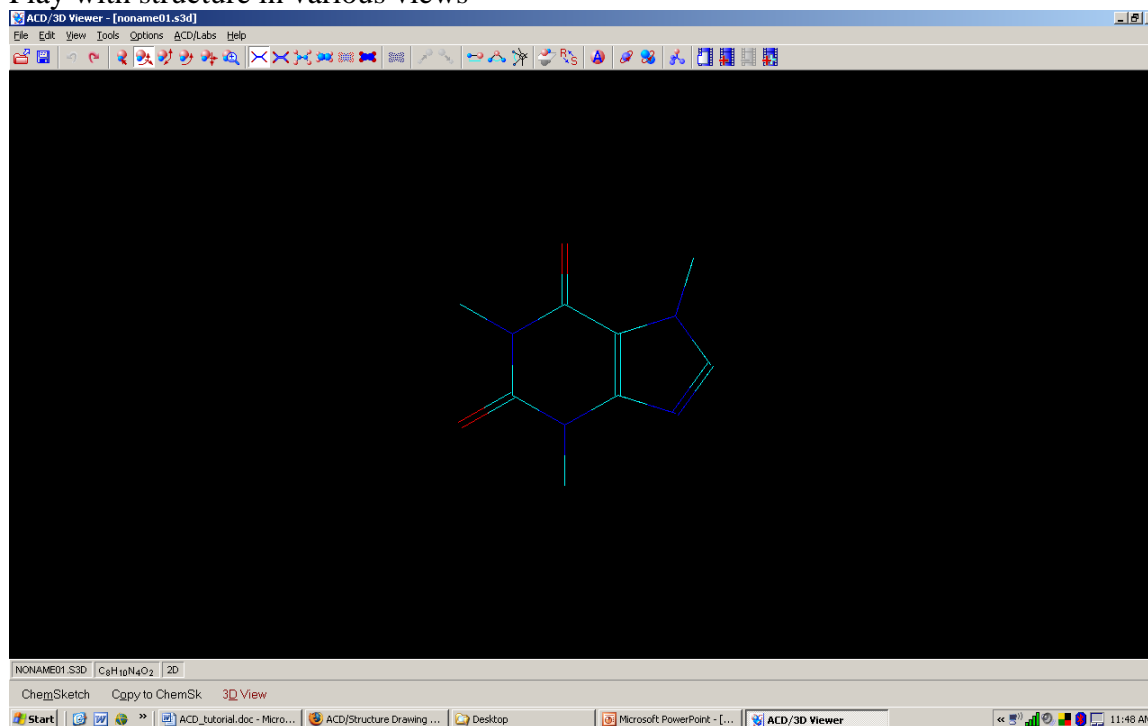


3D viewer:

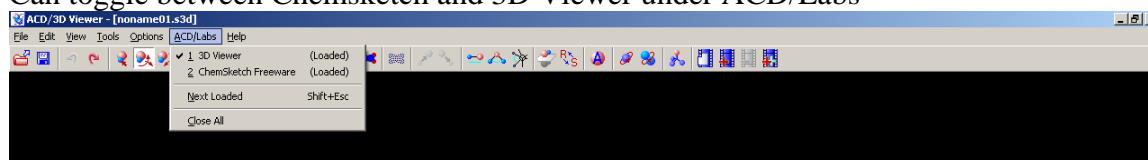
Click on "3D Viewer"



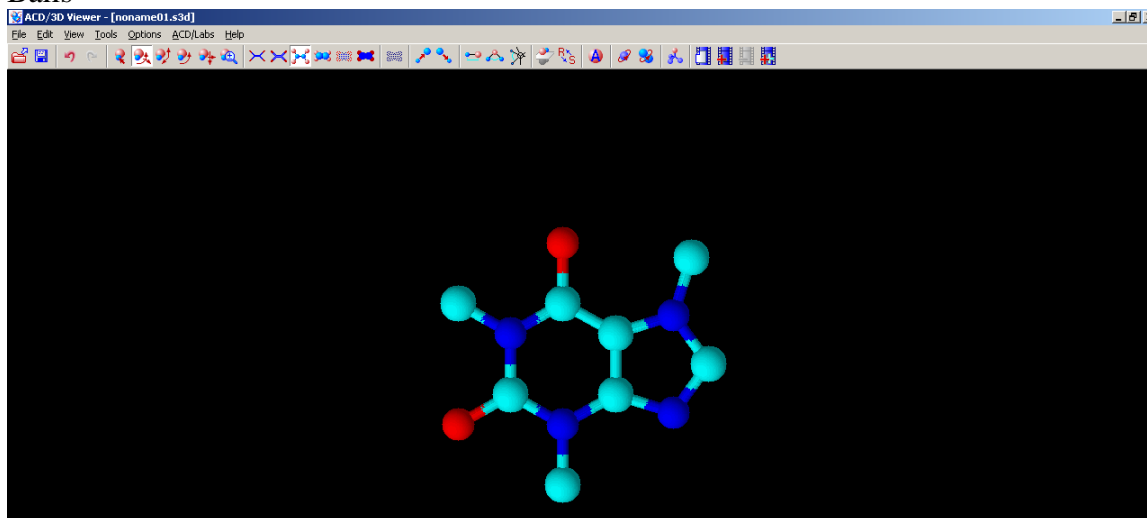
Play with structure in various views



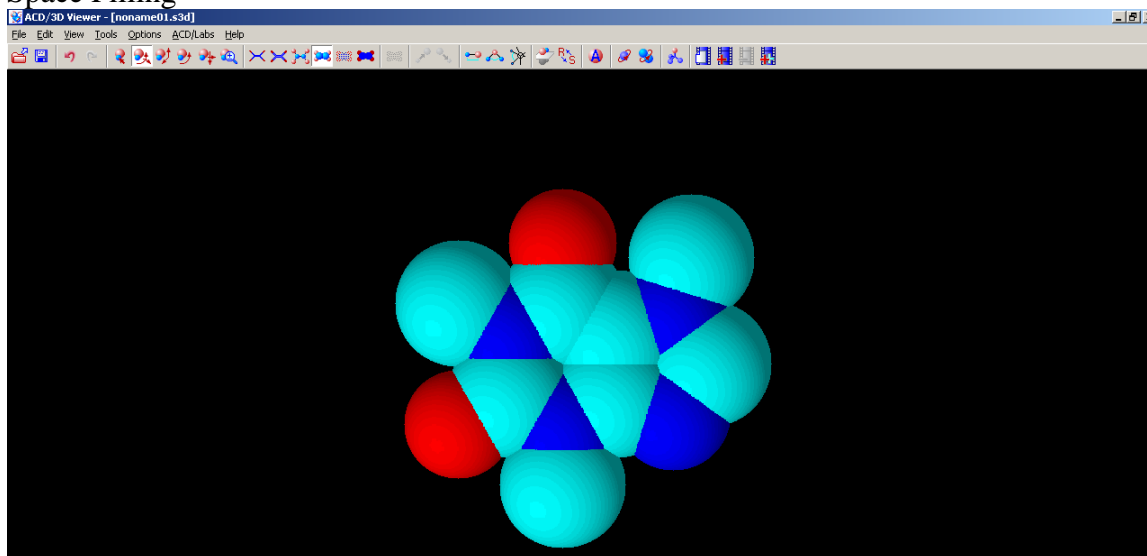
Can toggle between Chemsketch and 3D Viewer under ACD/Labs



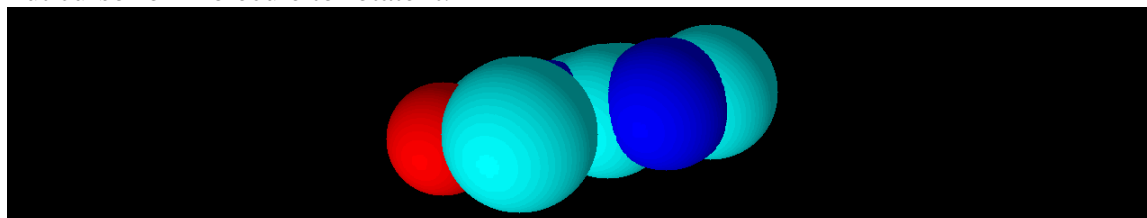
## Balls



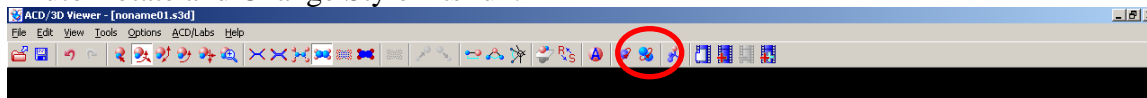
## Space Filling



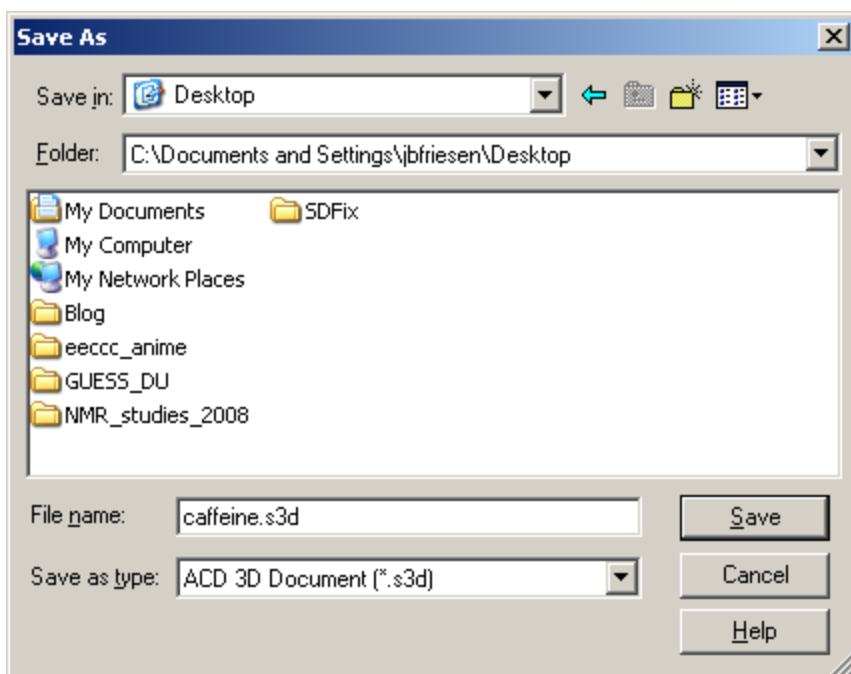
Put cursor on molecule to rotate it.



“Auto Rotate and Change Style” its fun.

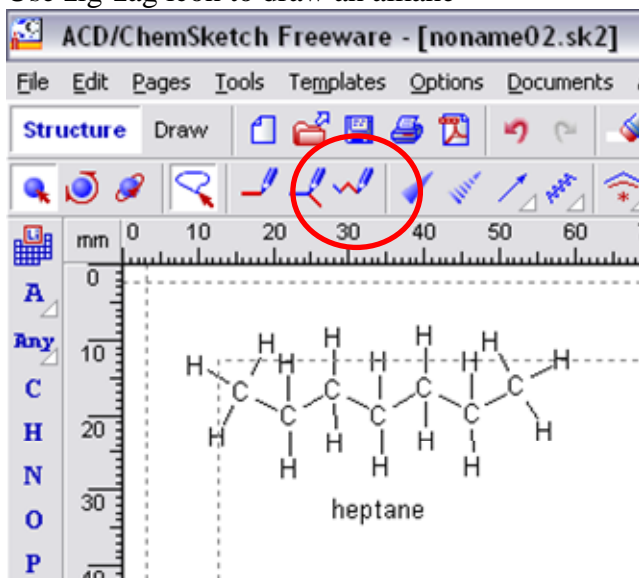


Can save it as a .s3d file

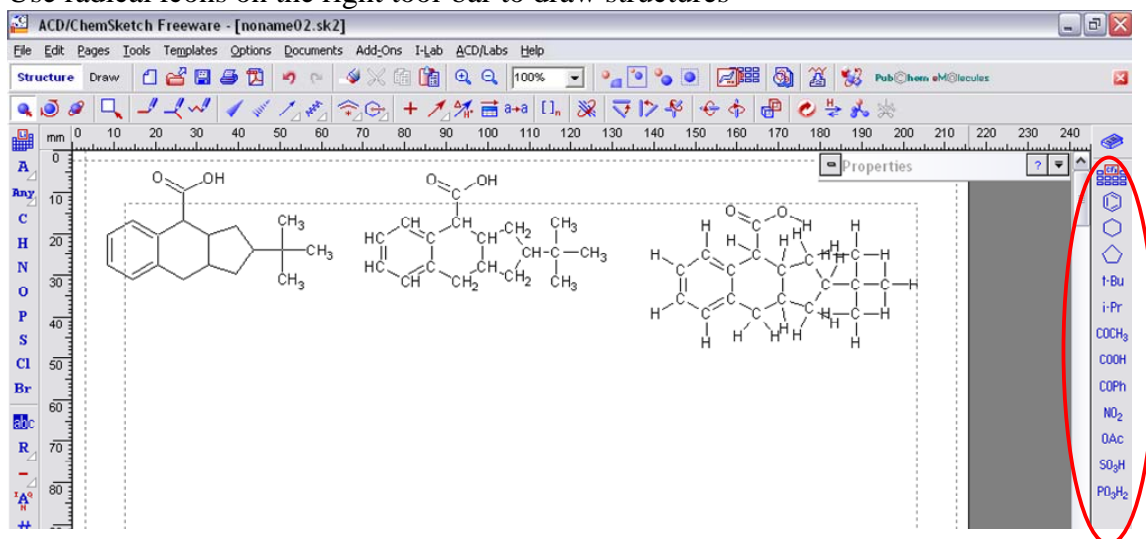


More drawing stuff:

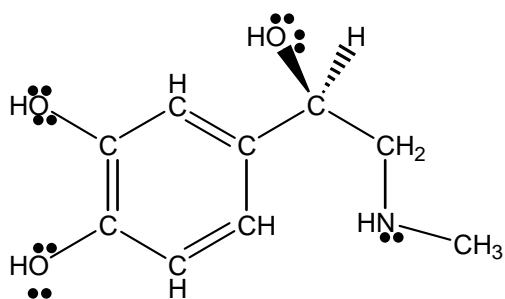
Use zig-zag icon to draw an alkane



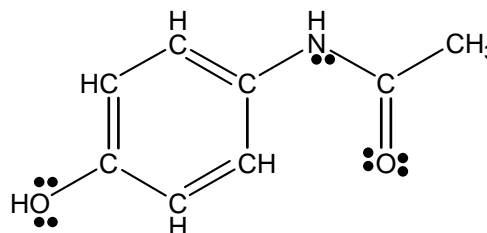
Use radical icons on the right tool-bar to draw structures



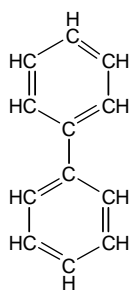
Other structure ideas:



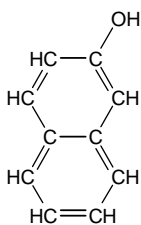
ephinephrine  
(adrenalin)



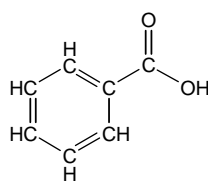
acetaminophen



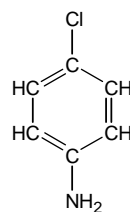
diphenyl



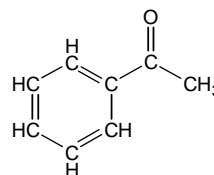
2-naphthol



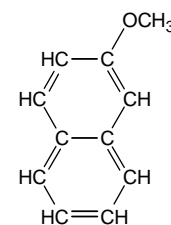
benzoic acid



4-chloroaniline



acetophenone



2-methoxy  
naphthalene