

Introduction to ChemSketch

ChemSketch is a free download for educational use. It can be used to produce structures of organic molecules, names of organic molecules as well as Lewis structures, 3D structures, space filling models or ball and stick models, among other things.

To get started go to

<http://www.acdlabs.com/download/chemsketch/download.html>

The screenshot shows the ACD/Labs website in a Mozilla Firefox browser. The page title is "Download ACD/Labs Freeware - Mozilla Firefox". The address bar shows the URL <http://www.acdlabs.com/download/>. The website header includes the ACD/Labs logo and navigation links: Products, Solutions, Support, Online Services, Resources, Downloads, Events, About Us, and Contact Us. The main content area is titled "Downloads" and features a sidebar with links to "Free ChemSketch Campus-wide Licenses for Academia", "Commercial ACD/ChemSketch", "ACD/Labs Online: per-pay and free access to predictions and databases", "Tools for Academia", and "Tell a Friend About ACD/Labs Freeware". The main content area lists "FREWARE* (available for personal home and educational usage only)" and "ACD/ChemSketch Freeware 12.0". It includes a list of included software: ACD/LogP Freeware, ACD/ChemBasic, and ACD/Column Selector. A search bar is located in the top right corner.

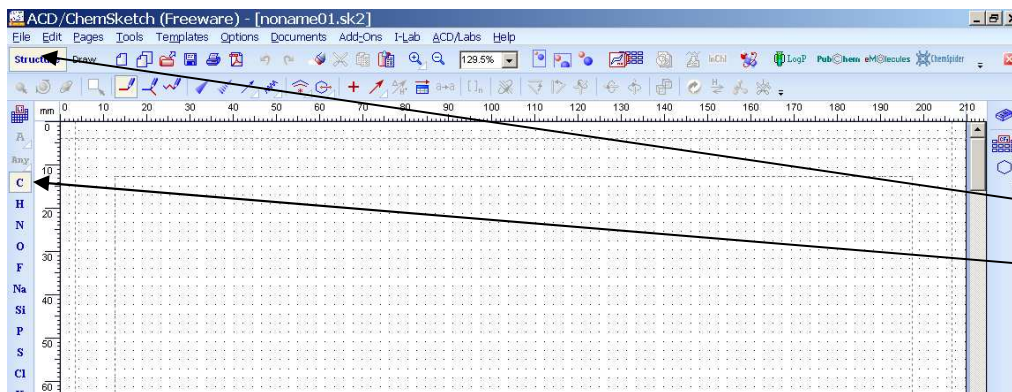
Select **ACD ChemSketch Freeware** and follow the instructions (an email address is required).

This is the latest version. (Periodically this is updated.) You do not have to work on-line to use the program.

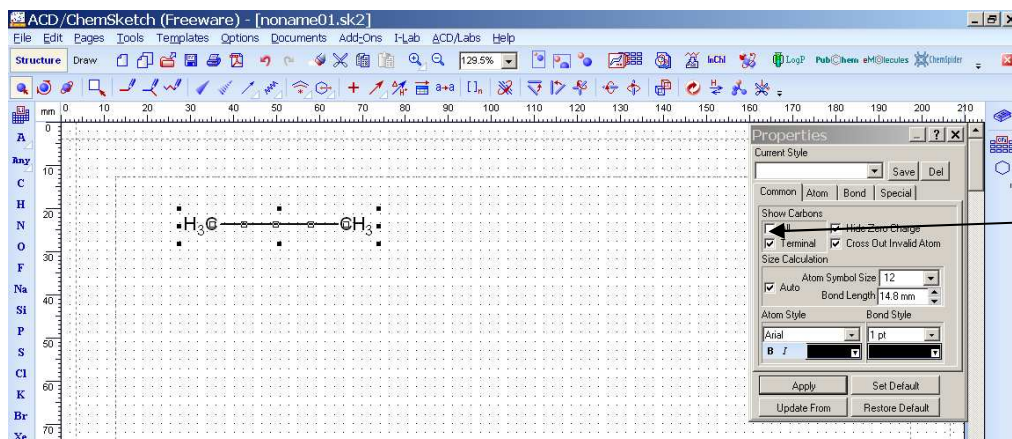
Using the buttons available. Note that a pdf document is part of the download.

The screenshot shows the ACD/ChemSketch software interface. The title bar reads "ACD/ChemSketch (Freeware) - [noname01.sk2]". The menu bar includes File, Edit, Pages, Tools, Templates, Options, Documents, I-Lab, ACD/Labs, and Help. The toolbar contains various icons for drawing and editing. The main workspace is a grid with a vertical periodic table on the left and a horizontal ruler at the top. Annotations with arrows point to specific features: "select" points to the selection tool; "select other elements from periodic table" points to the periodic table; "elements to select from" points to the periodic table; "undo" points to the undo button; "choice of arrows, including equilibrium arrows" points to the arrow tools; "change the way the bond appears - forwards (wedge) or backwards for a 3-D diagram" points to the bond style tools; "copy" points to the copy button; "paste" points to the paste button; "3D viewer" points to the 3D viewer icon; and "choose what you want to type" points to the text input field.

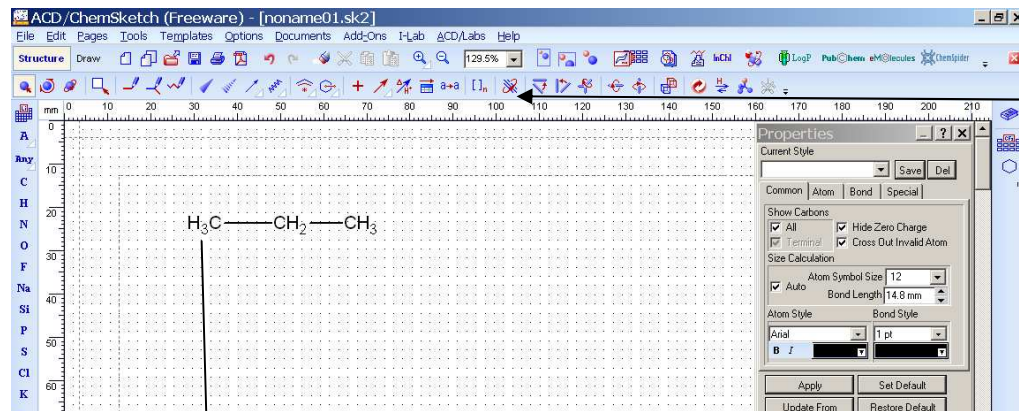
When you load the program this is what you will see.



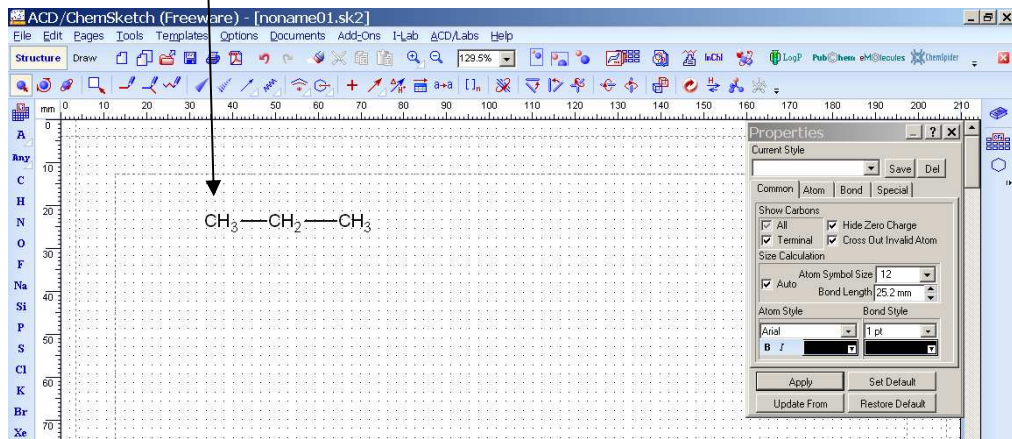
With structure highlighted, and C highlighted, you can draw a chain of carbon atoms.



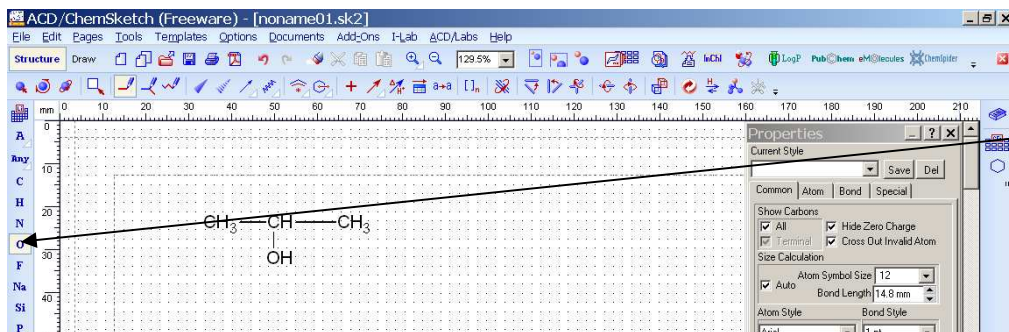
Select the whole structure by a lasso or clicking near the structure and select 'All' to show all carbon atoms, then 'Apply'. (Set default if you want to.)



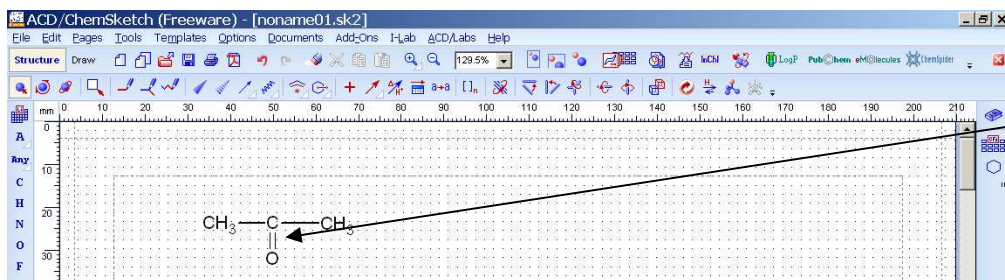
To have structure as CH₃ – rather than H₃C – , change position by clicking onto the 'change position' button, select the C atom that you want to change and click until you have the desired position.



Using the properties box you can change font size, etc. 'Lasso' what you want to change first using OR click next to the structure to select it.



To add, eg -OH groups click the atom (O if you want an -OH group) from the left hand side' select the carbon where you want this and drag out.



To make a double bond (or triple bond) select the bond to the OH group.

Using Tools options

The screenshot shows the ChemSketch interface with the 'Tools' menu open. The menu items and their keyboard shortcuts are:

- Structure Properties (Alt+Shift+S)
- Clean Structure (F9)
- Check Tautomeric Forms (Ctrl+Shift+T)
- 3D Structure Optimization (Ctrl+Shift+3)
- MassSpec Scissors
- Show Aromaticity (Ctrl+Shift+A)
- Hide Aromaticity (Ctrl+Shift+H)
- Expand Shorthand Formulae (Ctrl+Shift+F)
- Add Explicit Hydrogens (Ctrl+Shift+Y)
- Remove Explicit Hydrogens (Ctrl+Shift+R)
- Bring Bond(s) to Front (Ctrl+F)
- Send Bond(s) to Back (Ctrl+K)
- Auto Renumbering (Ctrl+Shift+N)
- Clear Numbering (Ctrl+Shift+L)
- Generate
- Search for Structure... (Ctrl+Shift+C)
- Calculate

Annotations in the image:

- An arrow points from the '3D Structure Optimization' menu item to a text box: "use if you want to create a 3D molecule".
- An arrow points from the 'Generate' menu item to a text box: "use to name the structure".

Using 3D models of molecules

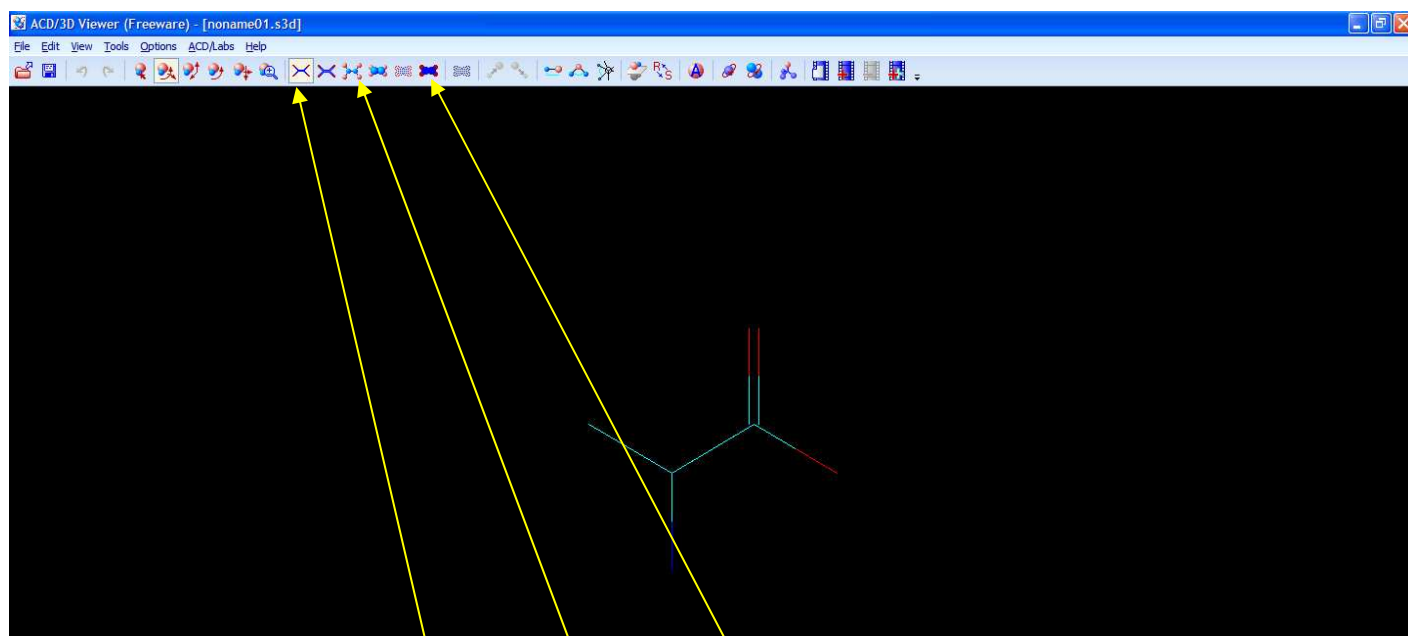
Draw, or get structure of molecule eg using alanine

When changing to 3D mode there are two possible ways to do this:

- (i) when you only have one molecule shown
- (ii) when you have more than one molecule in your chemsketch document.

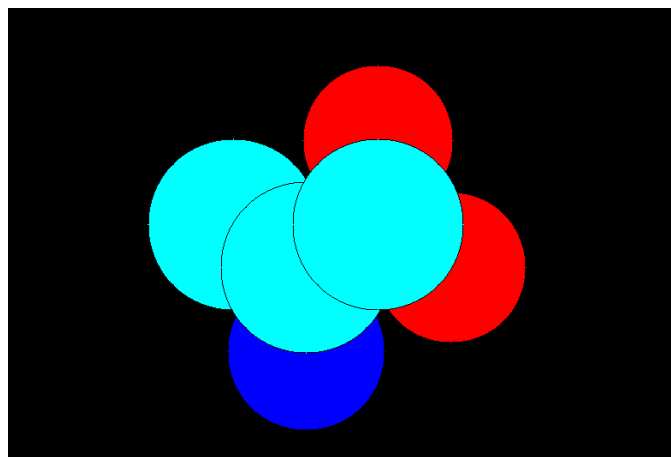
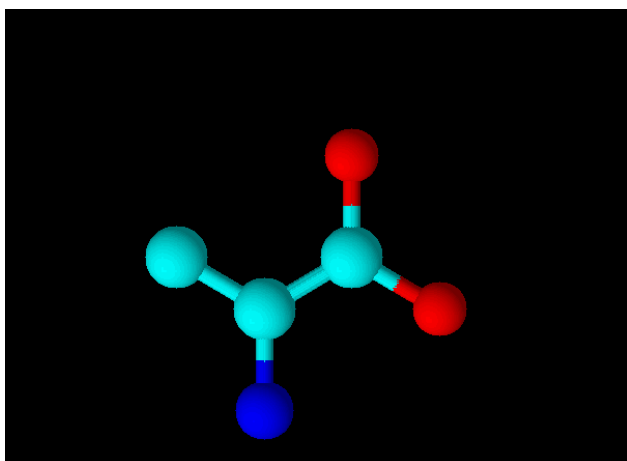
(i) when you only have one molecule shown

Select the molecule by clicking near it. Click the 3D viewer button (right hand side of buttons).

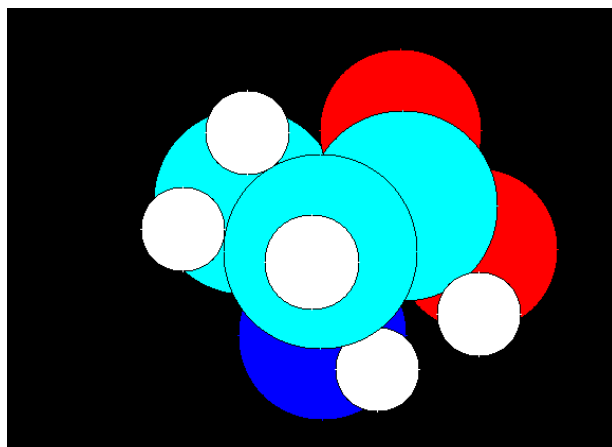
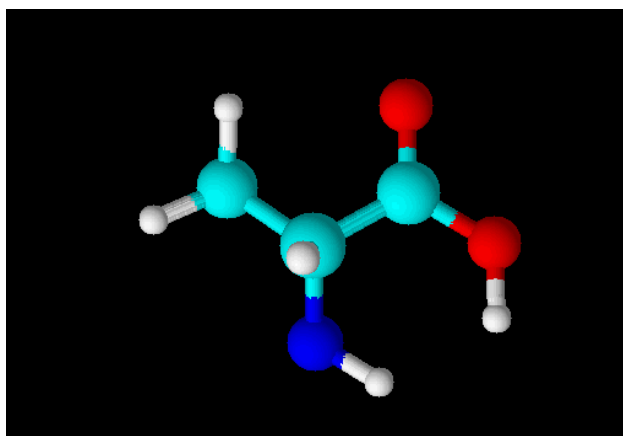


In 3D mode you can select framework, ball and stick, space-filling, etc.

eg

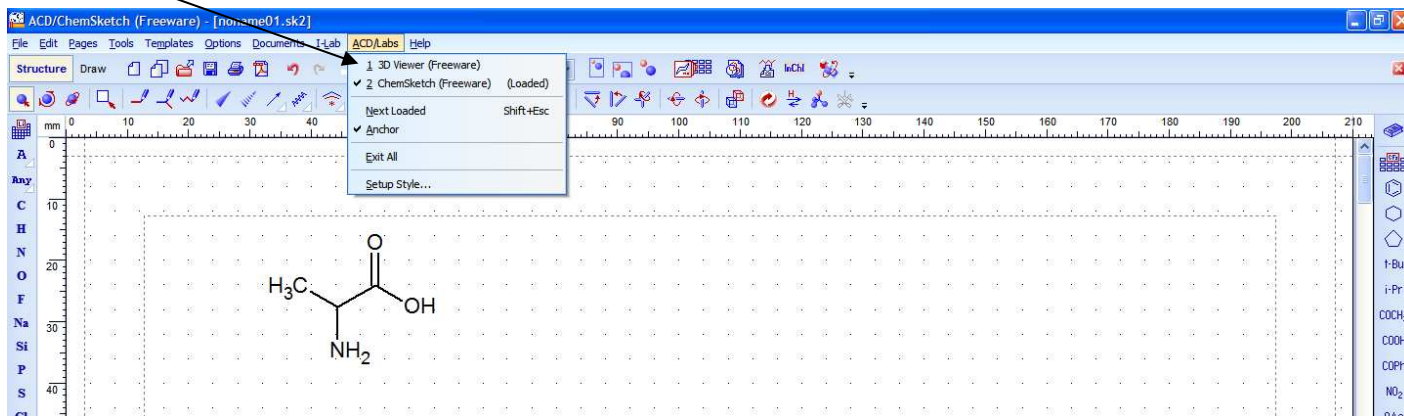


If you want to see all the hydrogen atoms, select the molecule and click onto **3D structure optimization** in **tools** before going to the 3D model.

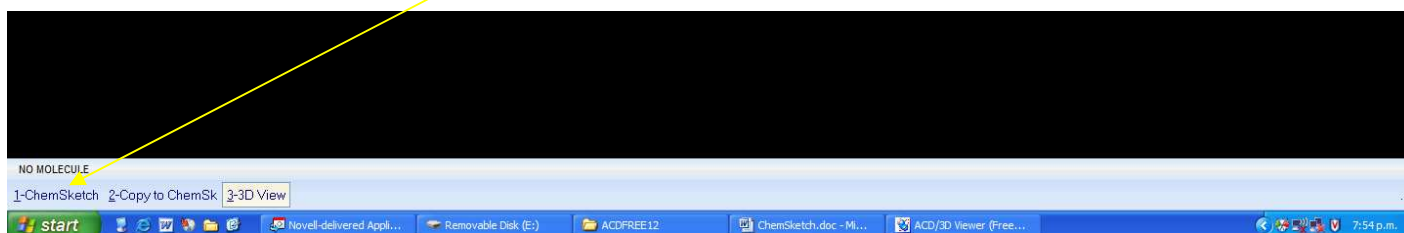


(ii) when you have more than one molecule in your chemsketch document.

Select 3D view from ACD labs. This will give you a blank screen in 3D mode.

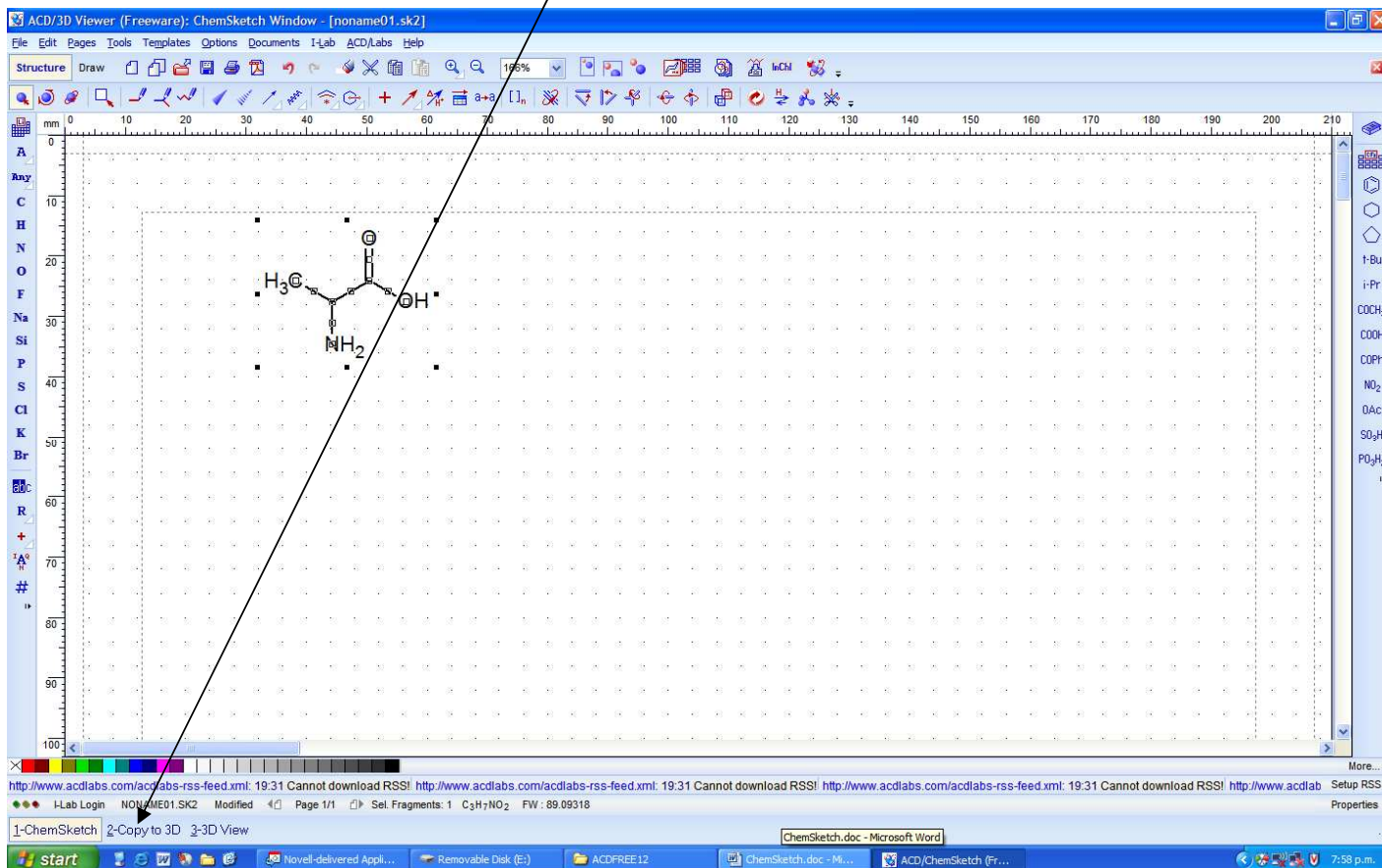


Select 1-ChemSketch bottom left of screen.



This takes you back to your chemsketch document.

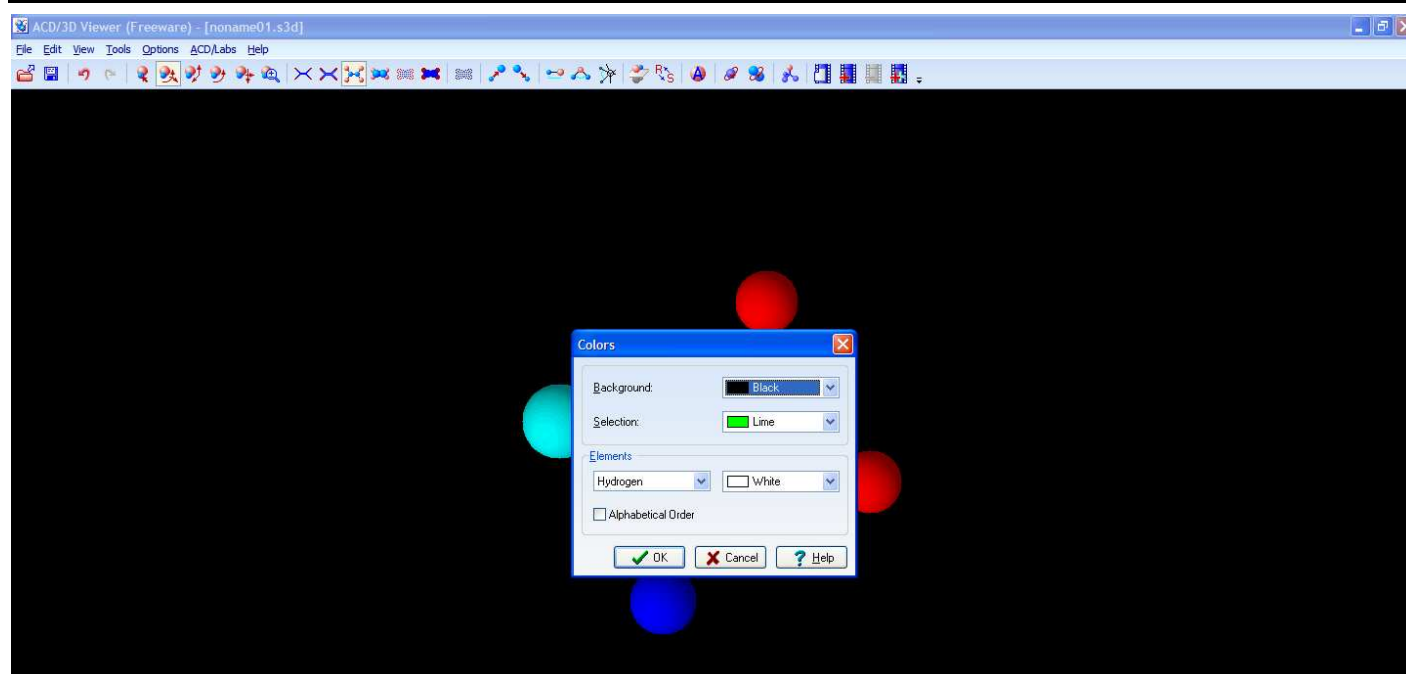
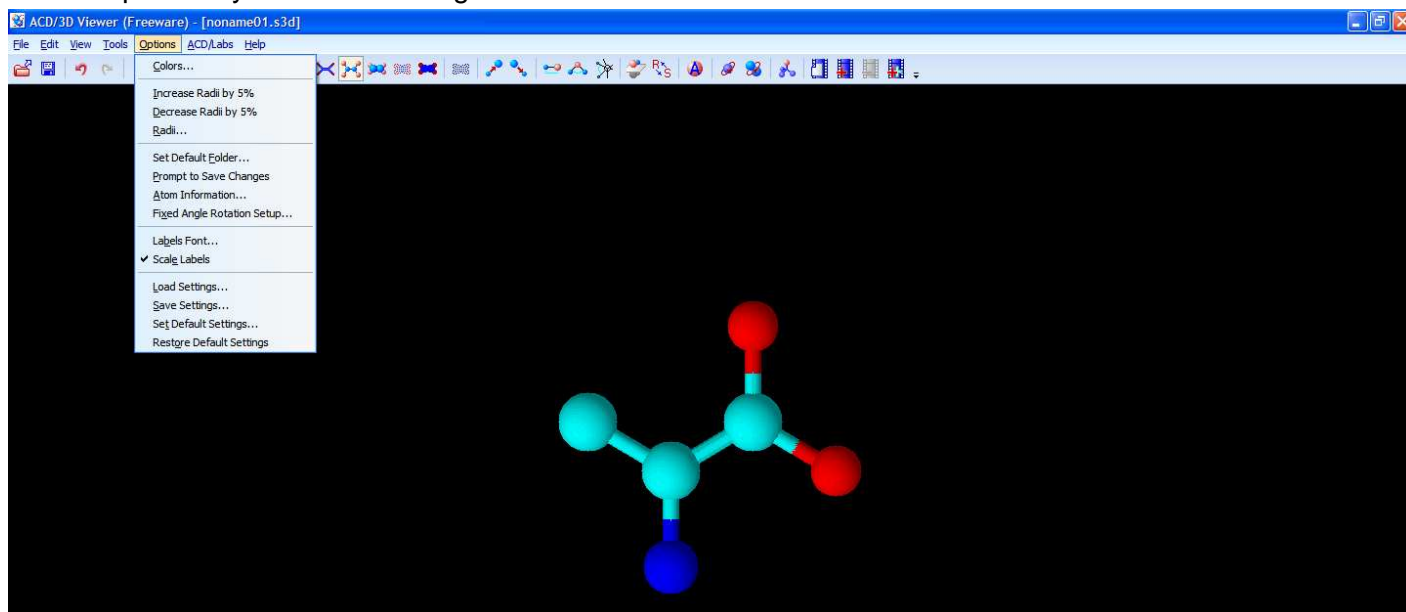
Then select the molecule and select Copy to 3D.



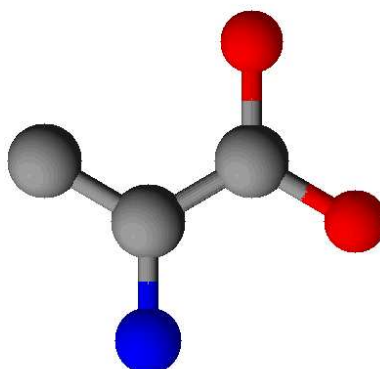
The molecule first appears as a frame work and you can change into the form you want such as ball and stick model or space-filling model, etc.

Using this method you can have a number of molecules on your page and select them separately to put into 3D. eg You could have *cis*- and *trans*- isomers that you could compare.

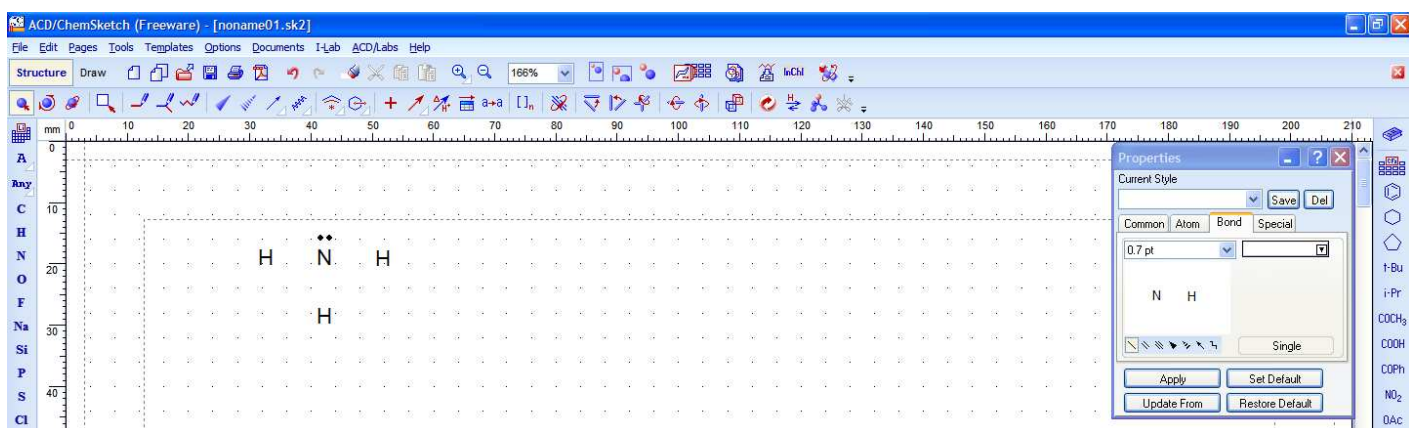
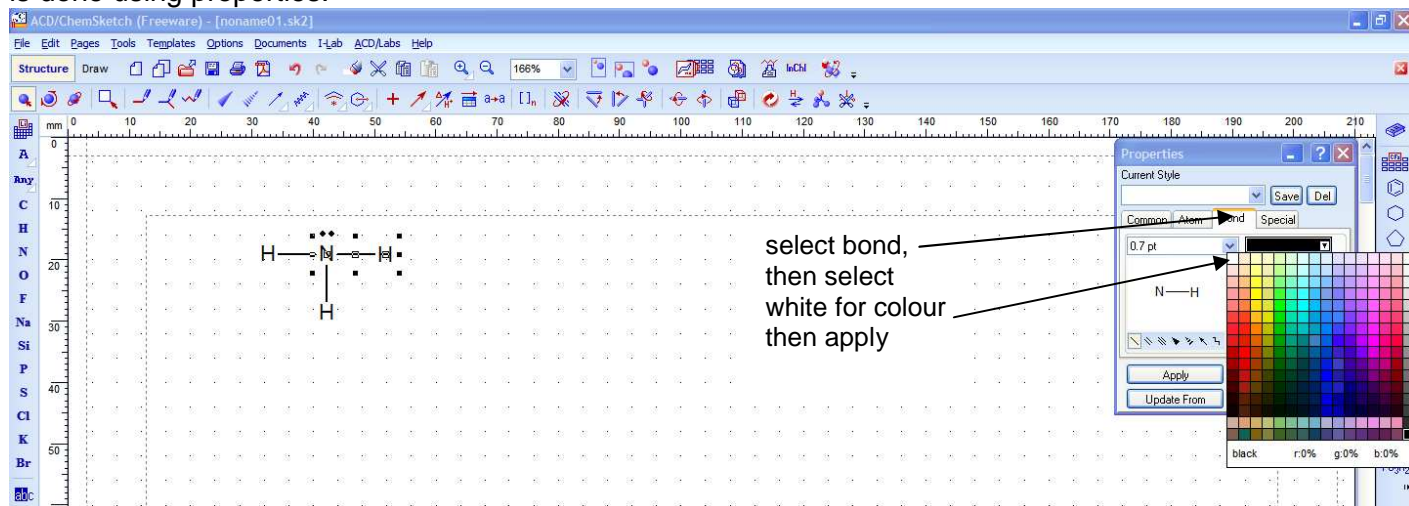
When you are in 3D mode you can use the mouse to move the molecule around to different views. You can change the colours and copy the molecule into other documents. Select Options if you want to change the colours used.



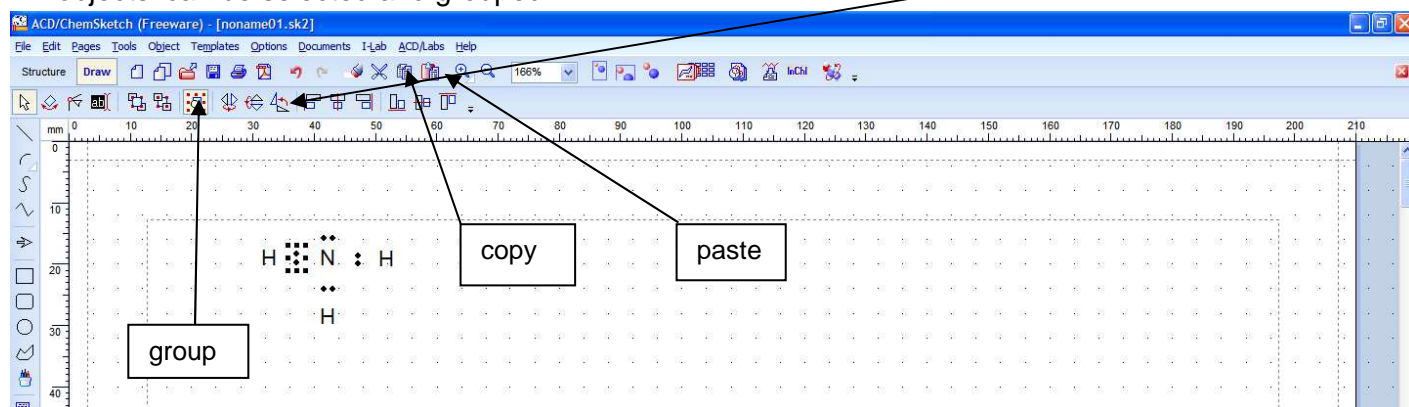
eg Make the back ground white, carbon black, oxygen red, nitrogen blue and hydrogen white.



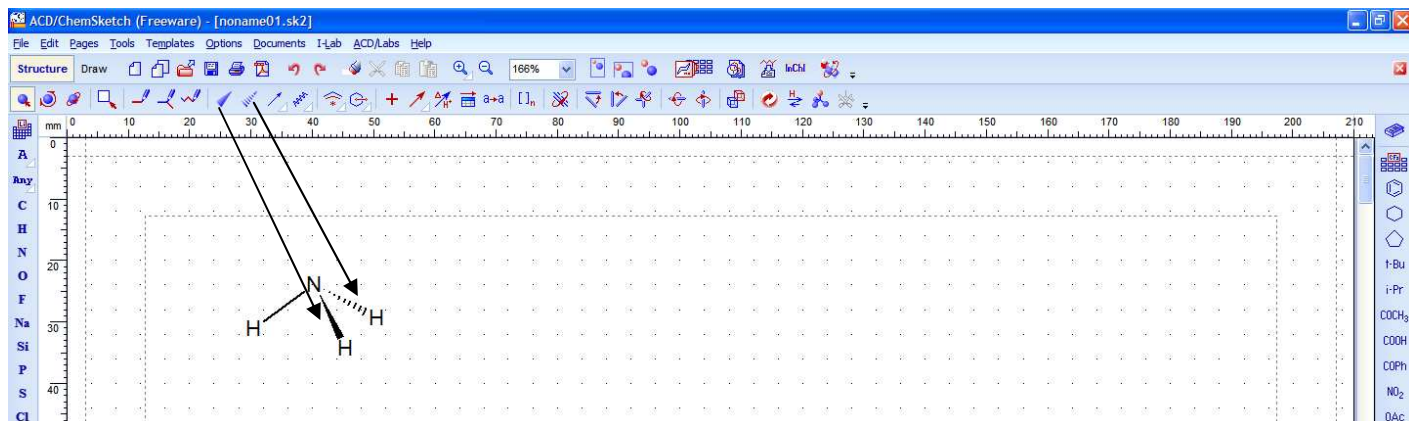
If you want to show all the bonds using dots, the bonds need to be change to white rather than black. This is done using properties.



Paste dots as required. This is done using draw. The dots may be moved through 90°. All 'objects' can be selected and grouped.



If you want to draw a 3D diagram rather than a Lewis structure, drag to the shape you want, select the 3D 'bonds' using the buttons at the top of the screen.



These are only some of the features that you will find useful from Chems sketch.

eg

You can select different arrows, including arrows suitable for equilibrium systems.

You can write reagents or conditions above the reaction arrow.

You can change an acid to the anion of the acid showing a negative charge.

Everything you do in Chems sketch can be copied into a word document.

The template window has a folder called lab kit which contains 7 pages of diagrams of equipment.

Once you get started you will find many other ways to use this programme so have fun!