Building interactive 3D organic molecules to use in Microsoft Office.

STANSW Workshop 2022
Presented by Dr Shane Wilkinson

Module 7: Organic Chemistry

HYDROCARBONS

Inquiry question: How can hydrocarbons be classified based on their structure and reactivity?

- Construct models identify the functional group and write structural and molecular formulae for homologous series of organic compounds up to C8: alkanes, alkenes, alkynes.
- Analyse the shape of molecules formed between carbon atoms when a single, double or triple bond is formed between them

Contents

Part 1: What's Needed

We will be using the freeware molecular modelling kit, Avogadro to build our molecules.

a) Install Avogadro: https://avogadro.cc/ (11 MB)

We will be using the freeware 3D graphics tool, Blender, to convert out molecules to digital 3D objects!

b) Install Blender: https://www.blender.org/download/ (214 Mb)

Whilst we wait for the downloads and installations, I will jump ahead to part 4 and show you the final product. All the assets are available to you in the Github to follow along!

Part 2: Building your molecules (in Avogadro)

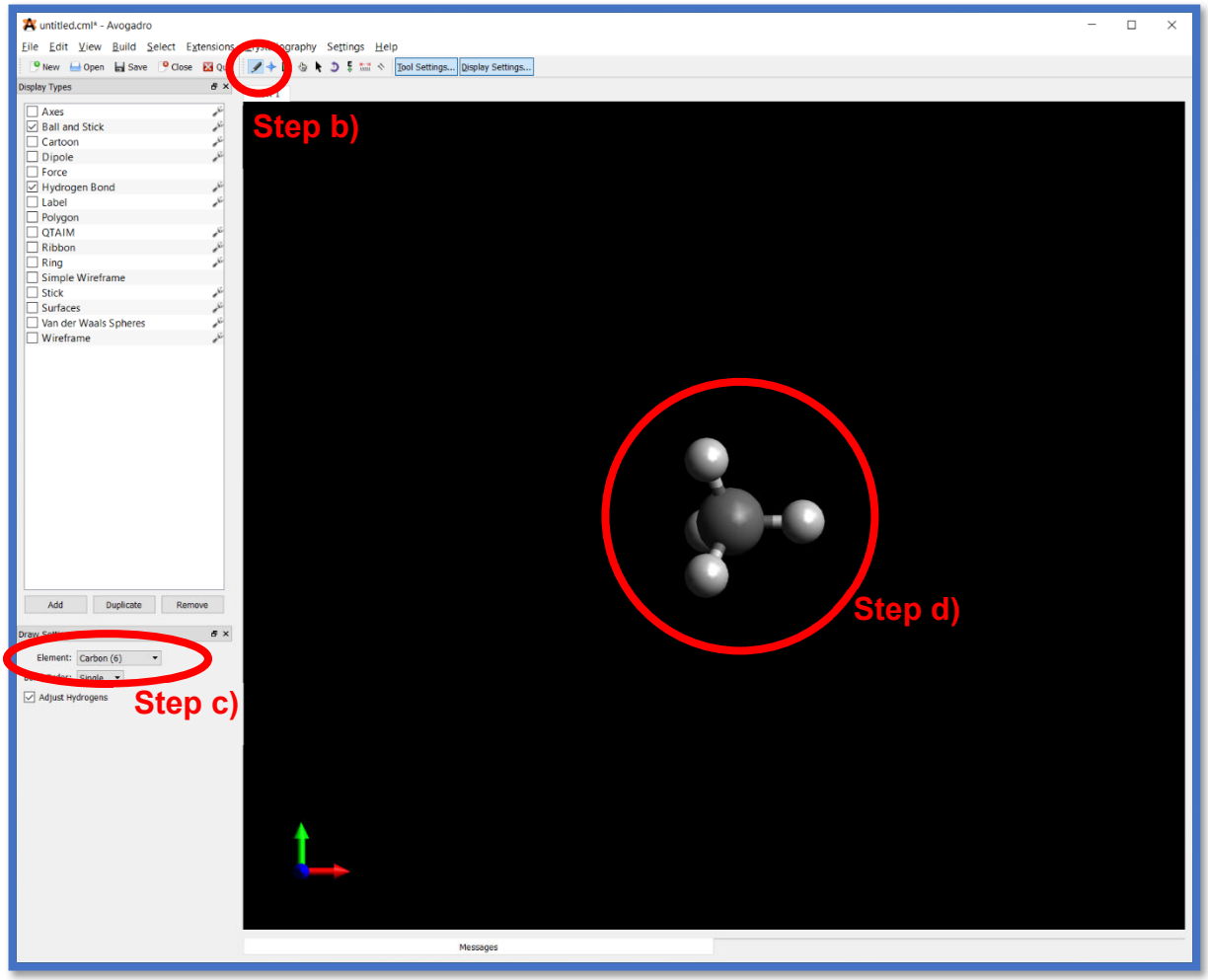
2.1 Building bonds

a) Open the Avogadro software.

b) Click on the build tool  *(It is likely already selected if you just opened the software)*

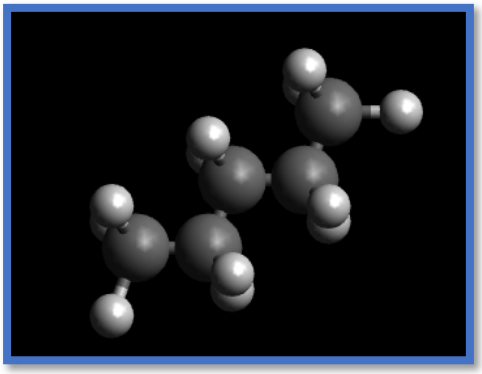
c) Change the element to “Carbon (6)” from the dropdown menu under Draw Settings. *(It is likely already selected if you just opened the software)*

d) Add a carbon atom into the workspace to generate a methane molecule.



e) Click on one of the smaller hydrogen atoms to convert it to a methyl group to create an ethane molecule.

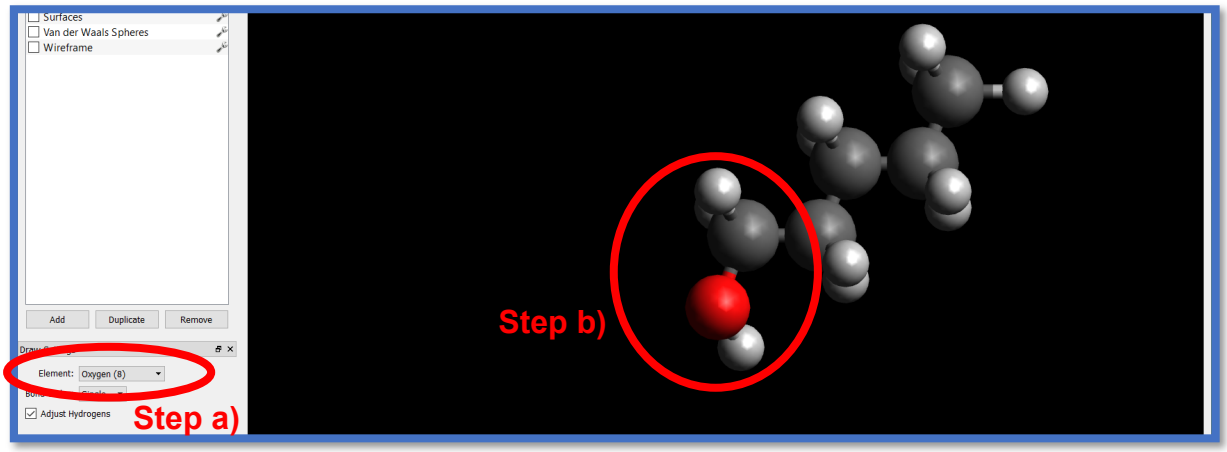
f) Repeat this three more times to create an unbranched pentane chain.



2.2 Changing atoms and bond order

a) Change the element to “Oxygen (8)” from the dropdown menu under Draw Settings.

b) Click on one of the terminal hydrogens and it will convert to an oxygen to generate pentanol.



c) Change the Bond Order to “Double” from the dropdown menu under Draw Settings.

d) Left-click+hold on the carbon you just added an alcohol. Drag the mouse just above the carbon and you should see a red atom with a double bond emerging from the carbon.

Don’t worry about the appropriate bond length or angle just yet, we will fix that later.

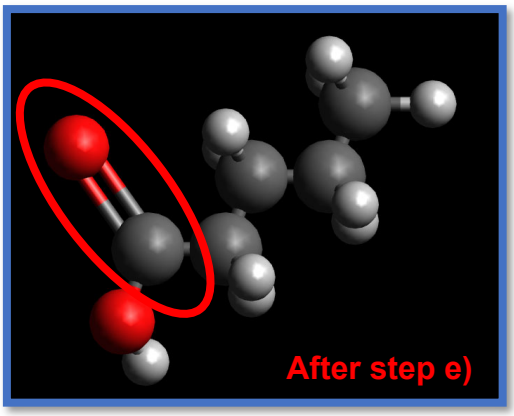
e) Release the mouse button and the newly drawn carbonyl will replace the remaining two hydrogens on that carbon (to generate a carboxylic acid – pentanoic acid).

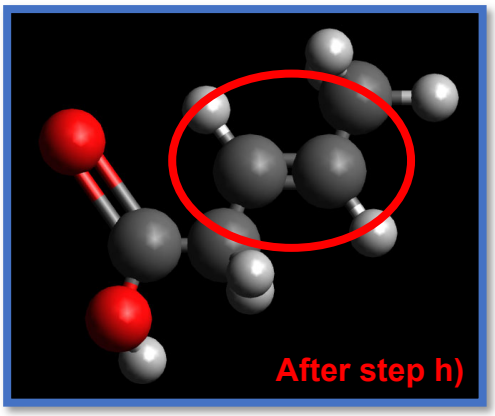
If you made a mistake, you can use ctrl+Z to undo any changes.

f) Change the element back to “Carbon (6)” but keep the Bond Order as “Double”.

g) Left-click+hold on the 3rd carbon and drag the cursor to the 4th carbon (from the carboxylic acid).

h) Release the mouse button and an alkene bond will be inserted (at the cost of two hydrogens) to generate pent-3-enoic acid).





2.3 Viewing your molecule

a) Click on the navigation tool .

b) Left-click+hold in the empty space and drag your mouse to rotate your molecule.

c) Left-click+hold on any atom and drag your mouse to rotate your molecule around this atom.

d) Use your scroll wheel (or centre-click+hold and drag) to zoom in and out of your molecule.

e) Right-click+hold and drag your mouse to move your molecule.

f) Double-click will reset views and centre your molecule.

2.4 Optimising bond lengths and geometry.

a) Click on the "Auto Optimisation Tool" .

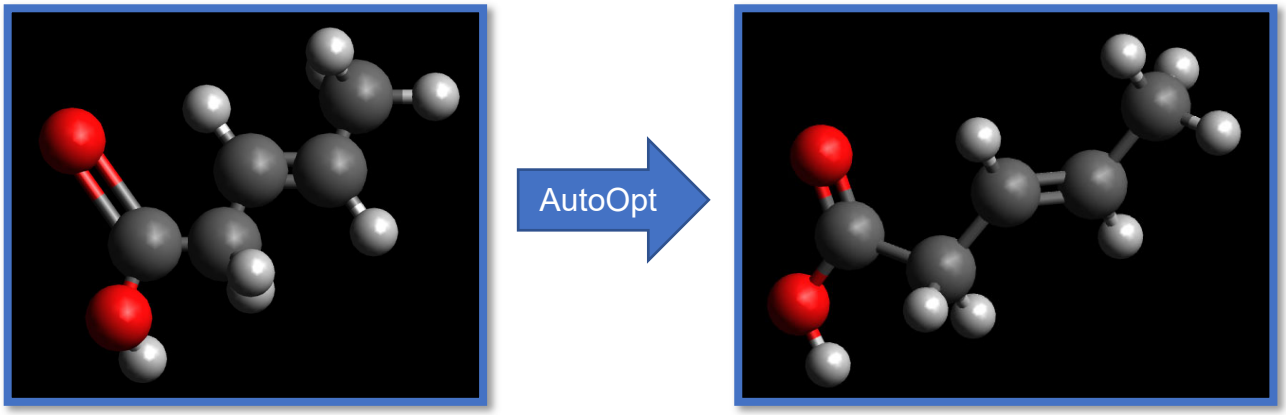
b) Change the Force Field to "MMFF94" from the dropdown menu under AutoOptimization Settings.

UFF *= Universal Force Field. This model can optimize the geometry for <u>all</u> elements, and does well with inorganic materials, and organometallic materials.*

MMFF94 *= Merck Molecular Force Field. This model specialises in the geometry and forces associated with organic compounds.*

c) Click "Start".

The molecule will re-shape to optimise bond lengths and angles. The energy of the molecule is displayed in the top-left corner of the workspace. Once it has found a minimum conformation, the change in energy (dE) shows a value of 0.*
** The minimum conformation may not be the LOWEST conformation achievable.*

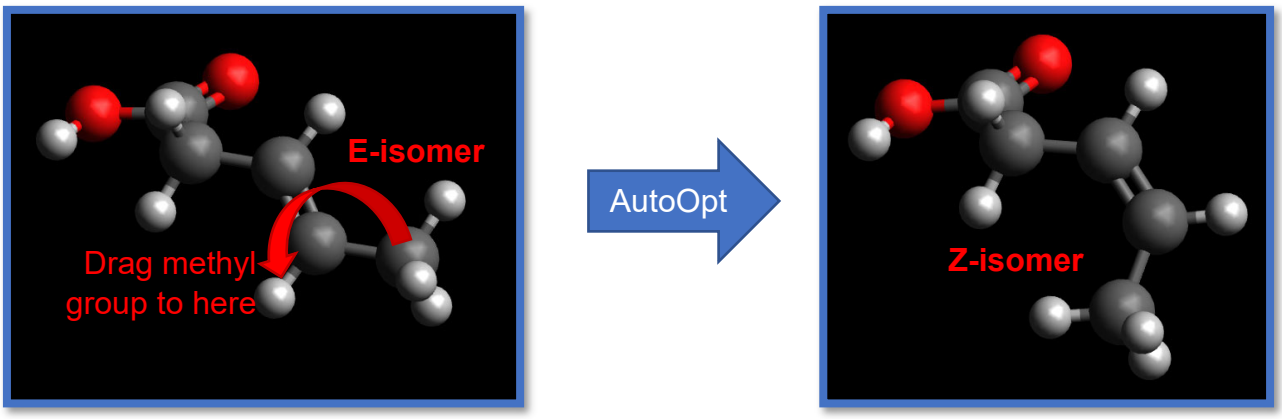


d) You can navigate around your molecule using steps 2.3b-f EXCEPT when you left-click+hold on an atom, you do not rotate around that atom, but instead drag that atom. Letting go will cause the molecule to re-optimise the bond lengths and angles once more. You can use this to influence certain conformations (step 2.4f).

Note details such as the staggered orientation of alkane chains.

e) Once your autoOpt has found its minimum (dE = 0), make a note of the AutoOpt E value for your molecule.

f) Grab the methyl group and drag it to the other side of its attached carbon to force the auto Optimization to optimise the Z-isomer. What is the energy of this molecule now?



g) Have a play at finding the optimised conformer or try and "break the molecule" and watch it re-optimise. You may need to "stop" the auto-optimisation if you wish to change multiple atoms before it starts optimising.

Things to explore:

- *Staggered vs eclipsed conformers: Make the methyl hydrogen eclipse the alkene hydrogen and then let it optimise to see which orientation is preferred.*
- *Does the acidic proton prefer to be facing away or towards the carbonyl oxygen. Why might this be?*
- Which is lower in energy? Having the carboxylic group eclipsing the alkene or off to the side?

h) Agree on a final conformation for your molecule to use in the subsequent steps.

2.5 Measuring bond lengths and angles.

a) Click on the "Click to Measure Tool". 

b) Left-click on the carbonyl oxygen. A "*1" should appear on it.

c) Left-click on the carbonyl carbon. A "*2" should appear on it.

d) At the bottom-left of the workspace, the bond length should appear (~1.22 Å).

e) Left-click on the second oxygen (the OH). A "*3" should appear.

f) At the bottom-left of the workspace, a second bond length should appear (~1.35 Å) AND the bonding angle between the two oxygens.

g) Right-click to remove and reset the labelling.

h) Explore the bond-lengths and angles around your molecule.

2.6 Saving your molecule.

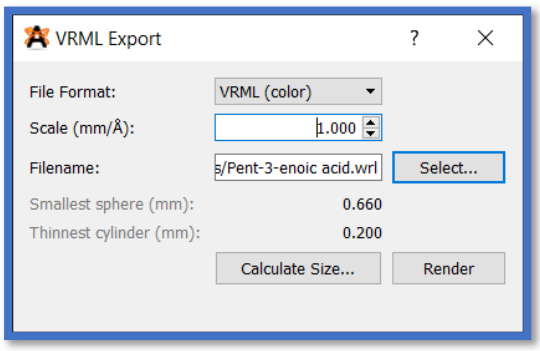
a) Click Save to save your molecule in case you need to come back and edit it.

*Avogadro saves your file as a *.xyz file. Unfortunately, Blender does not recognise this filetype and we will need to export out molecule as a separate file.*

2.7 Exporting your molecule (for Blender).

a) From the top-menu, click “File” > “Export” > “VRML…”

A pop-up window like below should appear.



b) Click on “Select…” to choose your file location.

c) In the pop-up window, select your folder location and provide a filename.

d) Click “Save”.

The pop-up window will close but the VRML window will remain. It can also now be closed.

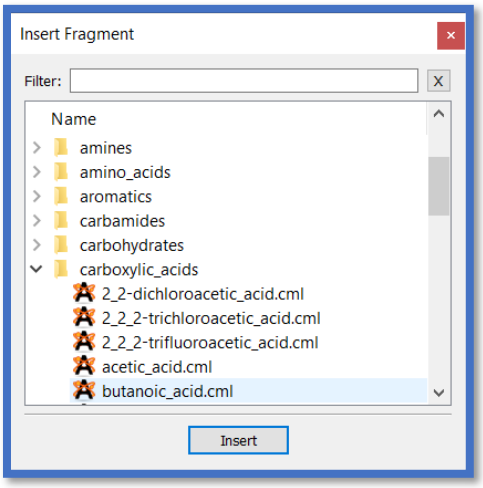
e) Close the Avogadro software. You are now ready to generate your 3D object in Blender (Part 3).

2.8 Pre-built molecules in Avogadro (Extension chapter)

a) Start a new workspace by clicking “Close”  on the top-left menu bar.

b) From the top-menu, click “Build” > “Insert” > “Fragment”.

A pop-up window will appear with folders for various functional groups.



c) Click on the arrow beside the folder to see what pre-built molecules exist in that fold.

d) Select on of the molecules and click “Insert”.

More than one molecule can be inserted at a time.

e) Close the pop-up window by clicking the red ☒ at the top-right of the window.

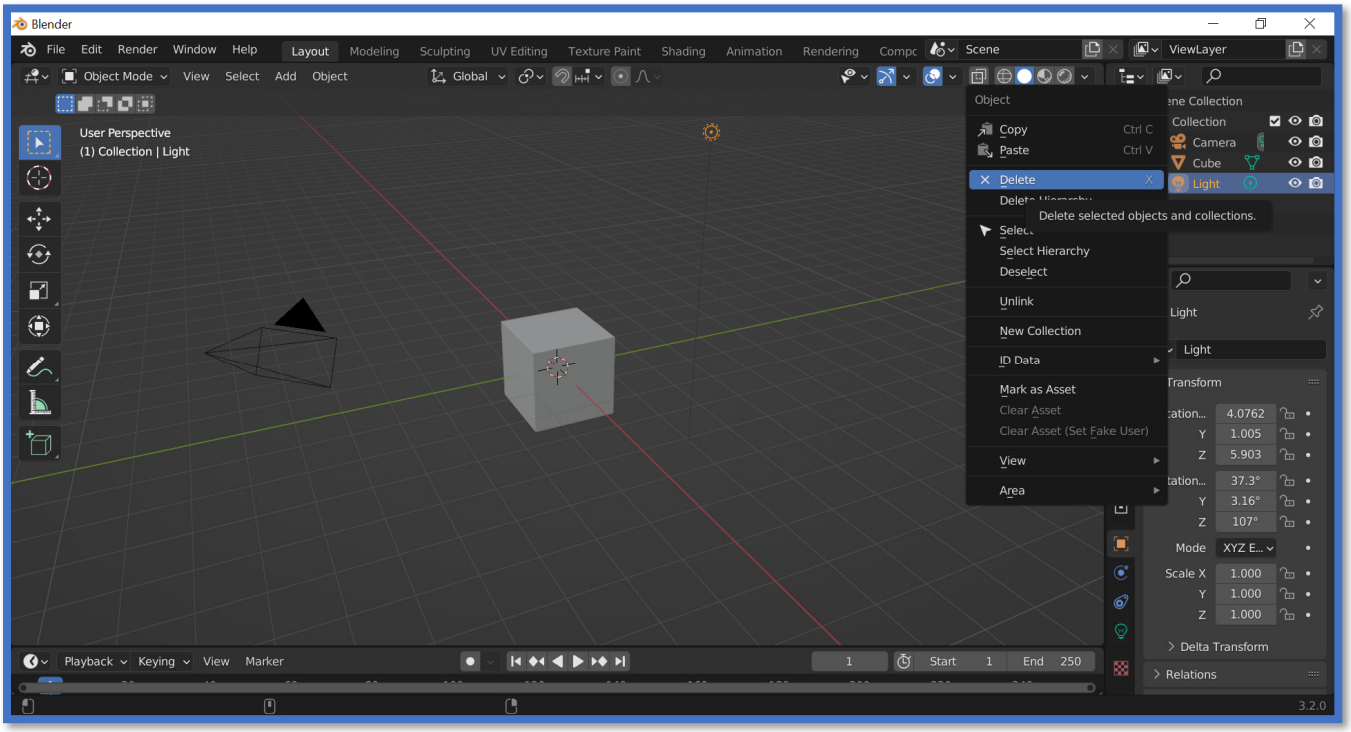
Part 3: Converting your molecules to 3D objects (with Blender)

3.1 Importing your molecule

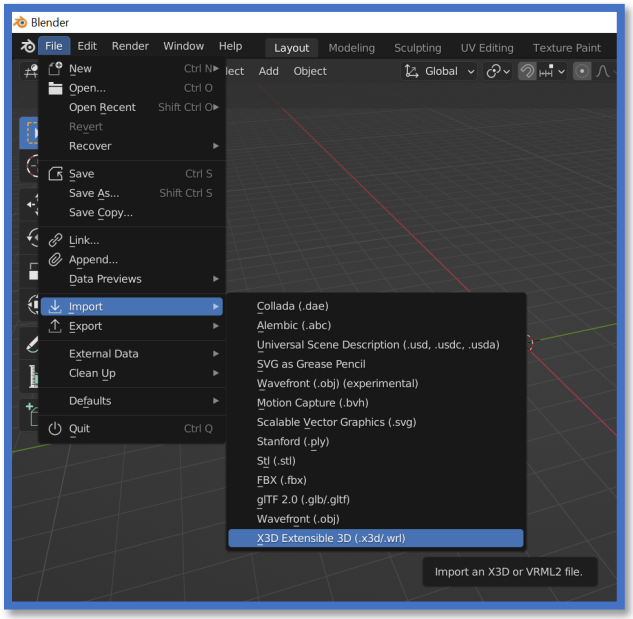
a) Open the Blender software (it can take up to 10 seconds to load).

b) Select “New File > General” from the pop-up window that appears.

c) In the top-right window, you can see the list of assets (camera, cube & light) in the workspace. Right-click on each and select “Delete” so we have an empty workspace.



d) From the top-menu, click “File” > “Import” > “X3D Extensible 3D (.x3d/.wrl)”



e) Locate your Avogadro export file (it’ll have a “.wrl” filetype).

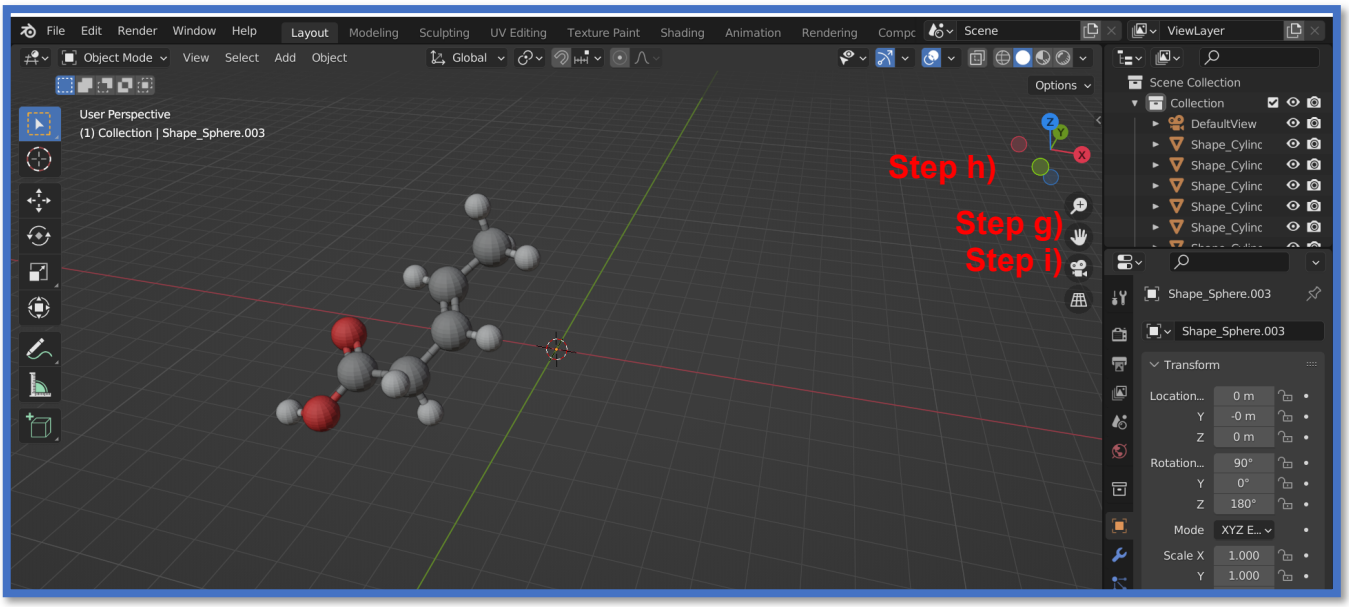
f) Click “Import X3D/VRML2”. Your molecule should appear in the workspace!

3.2 Navigating around your molecule.

a) Use the scroll wheel to zoom in and out (or left-click+hold the magnifying glass and drag your mouse).

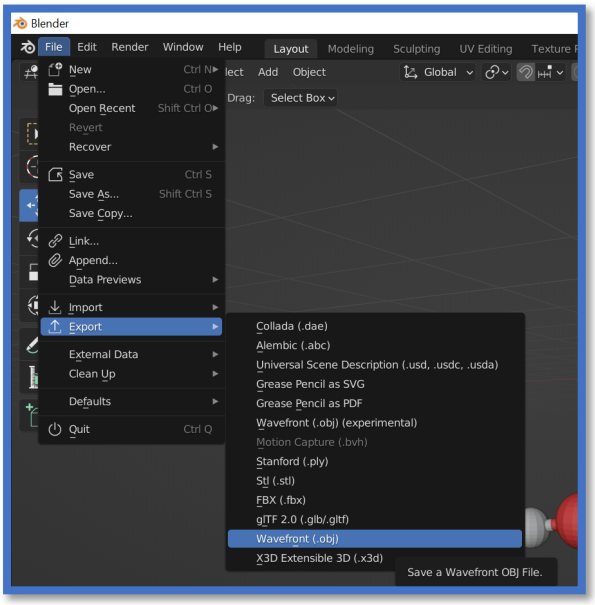
b) Left-click+hold the Cartesian Coordination axes and drag your mouse to rotate your molecule.

c) Left-click+hold the hand and drag the mouse to move the view.



3.3 Exporting your molecule

a) From the top-menu, click “File” > “Export” > “Wavefront (.obj)” (*Not the experimental one)*



b) Choose the file location you wish to save it and give it a filename.

c) Click “Export OBJ”.

d) DONE! You now have a 3D organic molecule that you can import into Office!

The following sections are if you wish to customise the surface and colour of your molecule.

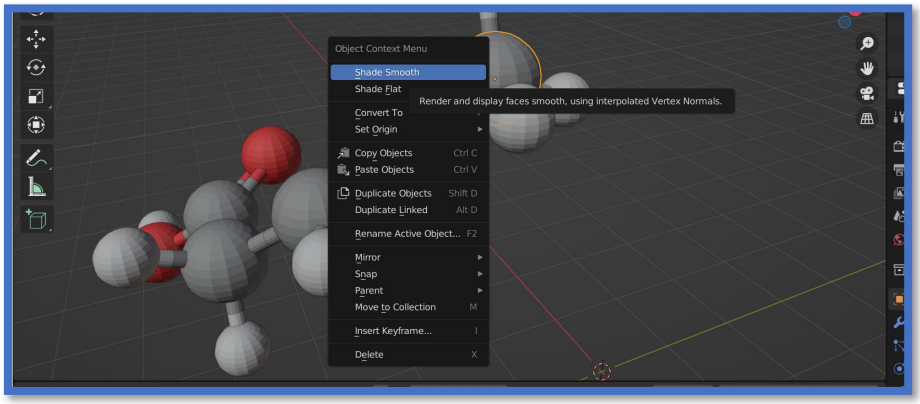
3.4 Changing the texture of the atoms (Extension).

By default, the atoms generated from Avogadro have a polygon shaped sphere. To smooth this surface:

a) Left-click on the atom you wish to smooth so it has an orange outline.

b) Right-click to bring up a menu bar.

c) Select “Shade Smooth”.



d) To revert back to the polygon effect, repeat and select “Shade Flat”.

3.5 Change the appearance (colour and sheen) of the atom (Extension)

I find the export from Avogadro results in a washed-out colour (especially carbon). We can re-colour our molecules in Blender.

a) First click on the “Viewport Shading” view in the top-right of the workspace.

This will show the end result after we modify the material properties.

b) Left-click on the atom you wish to change colour so it has an orange outline.

c) Left-click on the “Material Properties” icon (Red/pink checkerboard sphere).

d) Left-click on the “Base Color” bar to bring up a colour chart to choose from.

You can also use RGB, HSV or RGB colouring codes if you are familiar with them. Google CPK colours for atoms to find reference to their exact codes.

e) Left-click on the “Specular” value (it’s usually 0.5 by default).

f) Enter in a value of 0.2.

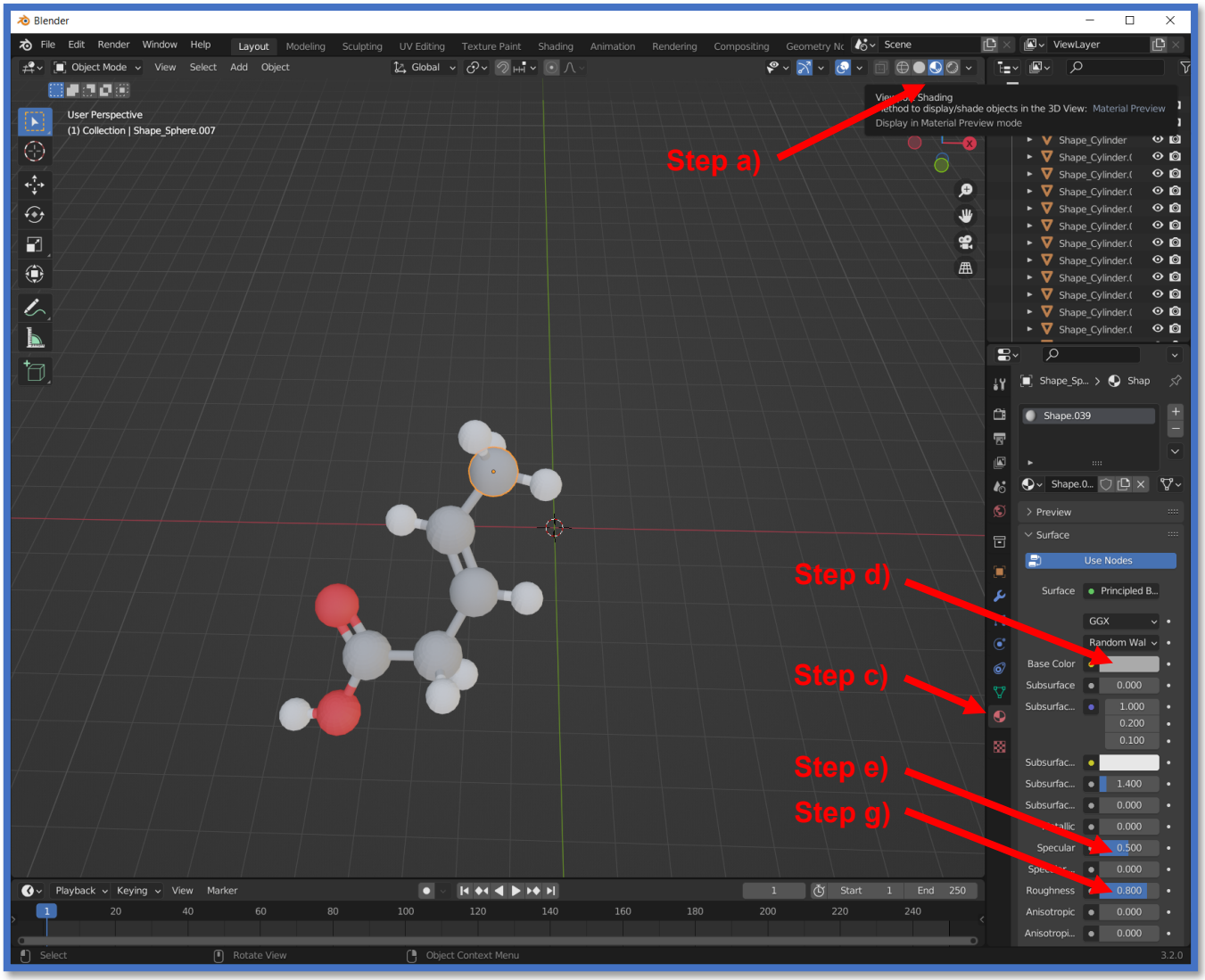
This value influences the “washout effect”. The higher the value, the more washed out it looks. However, I find a value of 0 is usually too saturated with colour. You can change this value to suit your liking.

g) If you want a reflective surface, on your atoms, left-click on the value for “Roughness” (it is usually 0.8 by default).

h) Change this value to 0.

You can choose any value (0 - 1) you wish depending on how glossy you want your atoms.

i) Repeat steps b-h for each atom you wish to change.



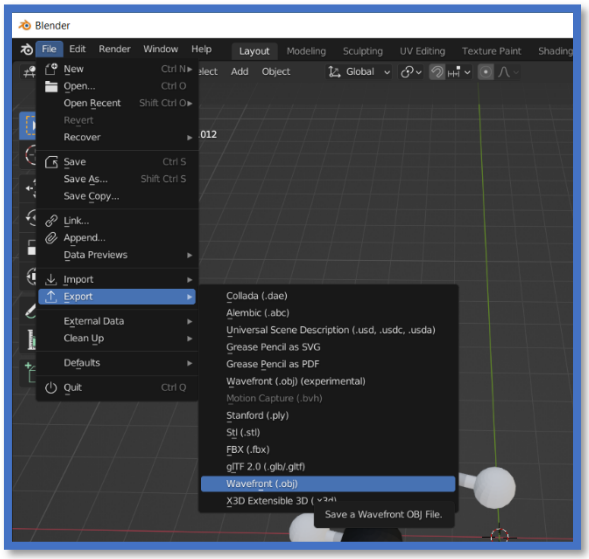
3.6 Exporting your molecule as a 3D object

a) From the top-menu, select “File” > “Export” > “Wavefront (.obj)”.

Don’t pick the experimental option.

b) Find a location to save your file and give it a filename.

c) Click on “Export OBJ”.



CONGRATULATIONS!

You have created a 3D object and are now a digital artist! Time to update the CV!

Part 4: Incorporating your 3D objects into Microsoft Office.

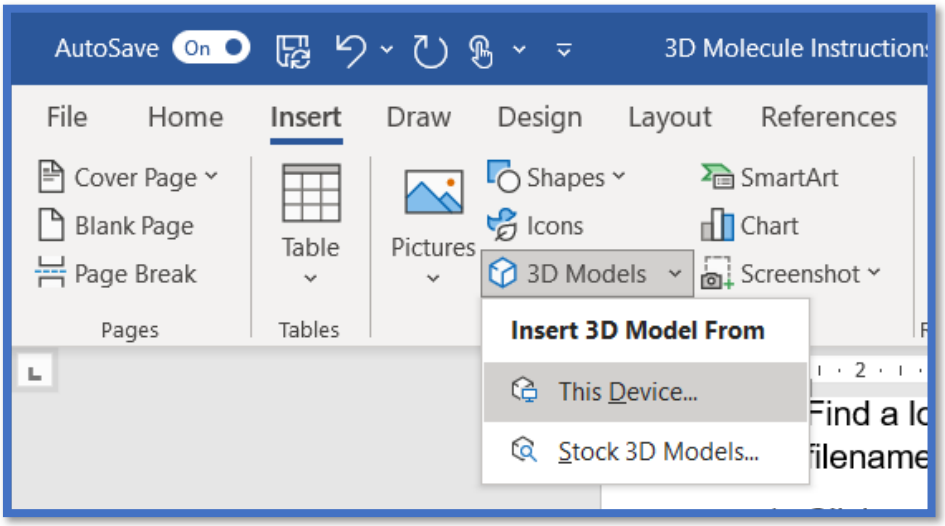
4.1 Incorporating 3D molecule into Microsoft Word

a) Place your cursor in your word document where you would like to place the 3D object.

b) From the top-menu, select “Insert”

c) Left-click on the down-arrow beside “3D Models”

d) Select “This Device…”.



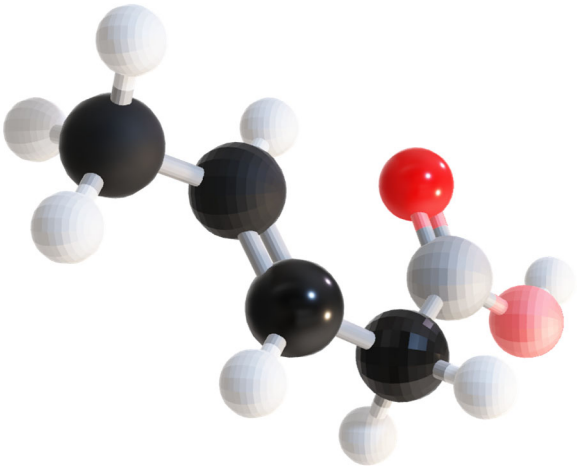
e) Navigate to your where you saved your 3D object (it’ll have the filetype .obj).

f) Click “Insert” and your 3D molecule will appear!

g) Re-size the object to fit your liking.

h) Left-click+hold the gyroscope icon in the centre of the molecule and drag your mouse to rotate your molecule in all three dimensions!

Tip: It’s best to display your molecule as “in front of text”. If you lock the molecule as “square” or “in line with text” it will cause your text to shift every time the molecule changes size/orientation.



4.2 Incorporating your 3D molecule into PowerPoint.

Unfortunately, the functionality isn't available for us to manually manipulate a 3D object DURING a presentation. But there are five animations specifically made for 3D objects that you can add to jazz up your presentations!

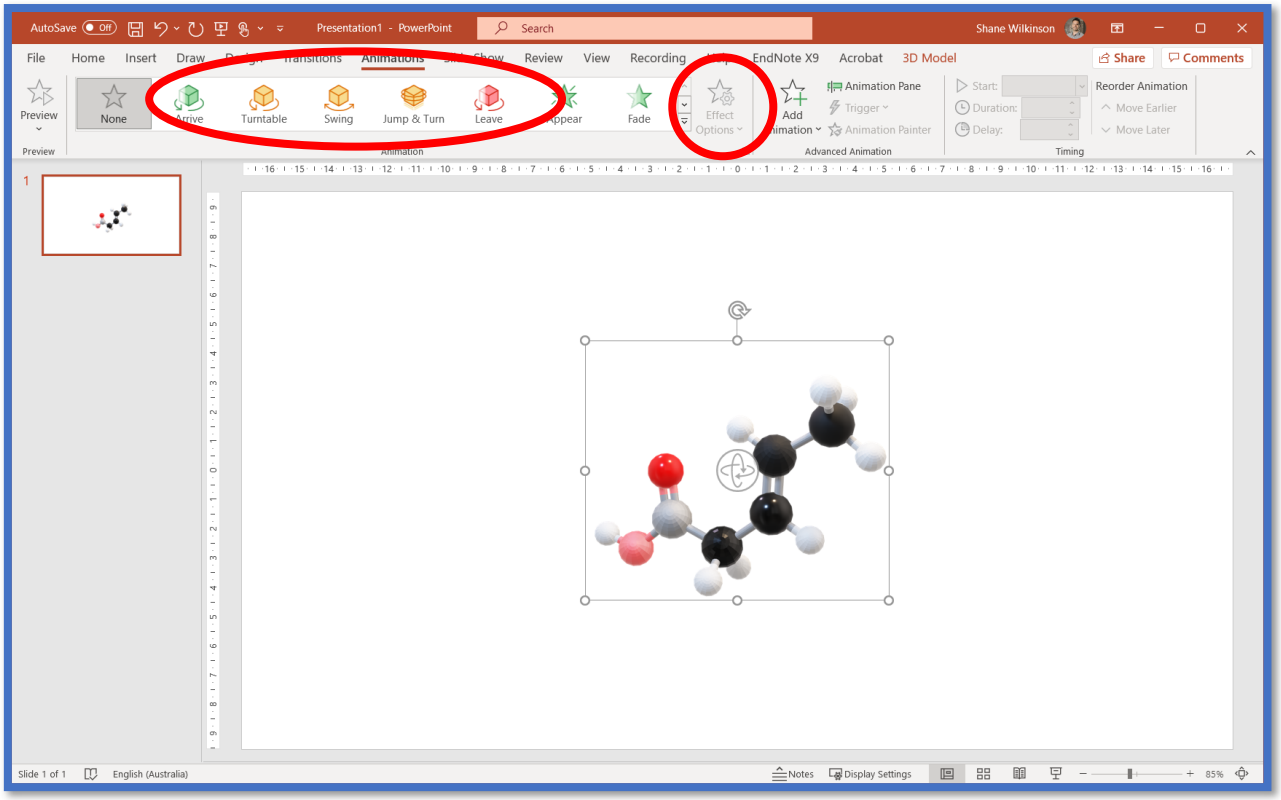
a) Insert a 3D object following the exact same steps above (4.1 b-h).

b) Position & rotate the molecule to how you want it to first appear in the slide.

c) From the top-menu, click "Animations".

d) Click "Arrive". *Your molecule will fade into view whilst rotating slightly into position.*

e) Click on "Effect Options" to customise the entry of your 3D object. Have a play with each option to see the effect.



f) Add an *additional* animation by selecting "Add Animation".

g) Choose one (or all) of the following animations and explore it's associated options from the "Effect Options":

- **Turntable**: Your molecule will do a full 360 spin
- **Swing**: Your molecule will pivot slightly in one direction, and then the opposite direction.
- **Jump & Turn**: Your molecule will seemingly do a summersault!
- **Leave**: Your molecule will turn and fade away as it exits your slide.

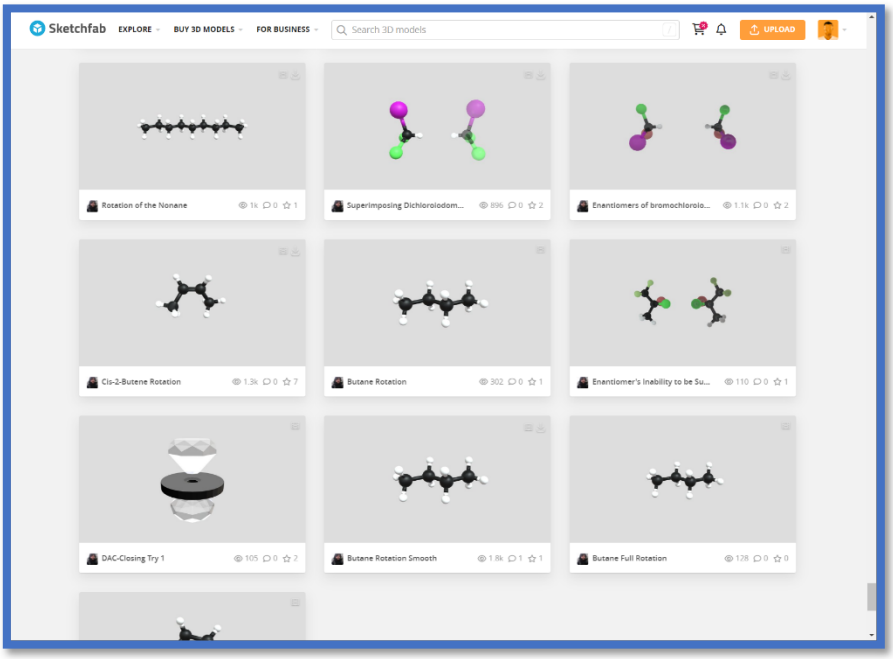
Tips: Use the "Animation Pane" to keep track of all the animations. You can also change the length of an animation and how it starts (ie click of the mouse or automatically).

h) Play your presentation in "Slide Show" mode to view your 3D molecule in action!

Part 5: Other resources for 3D models

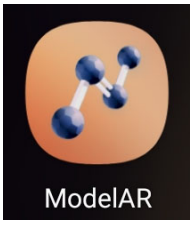
5.1 Sketchfab

https://sketchfab.com/



- This is a storage hub for 3D models that others have composed (some licensed, many free for educational purposes).
- Embedding codes are pre-coded if you use HTML or a Learning Management System (LMS).
- Make sure you download the .obj file if you wish to use the 3D molecules on offer. They should incorporate immediately into Microsoft Word and PowerPoint.
- Quite a few Chemistry Contributors (eg https://sketchfab.com/Michael.Aristov/models)

5.2 ModelAR:Organic Chemistry App by Alchemie



- Build organic molecules on your phone/tablet. Free and accessible modelling kits for students!
- Geometry generally well represented. Conformation energy isn't really considered. Fun to blow up the molecule when you're done.
- Available on iOS:https://apps.apple.com/au/app/modular-organic-chemistry/id1438760201
- Available on Android: https://play.google.com/store/apps/details?id=com.alchemie.modelset