Online virtual molecular modelling kits

STANSW Workshop 2022

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PART 1: Visualising Simple Organic Molecules

Module 7: Organic Chemistry

HYDROCARBONS

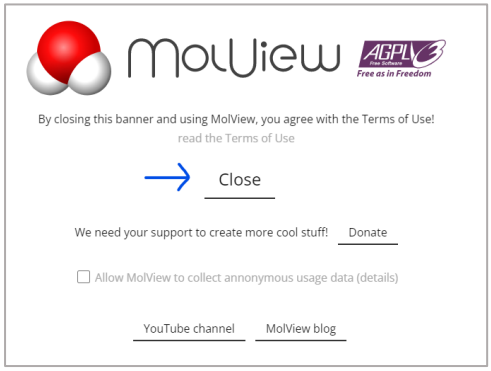
Inquiry question: How can hydrocarbons be classified based on their structure and reactivity?

- 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

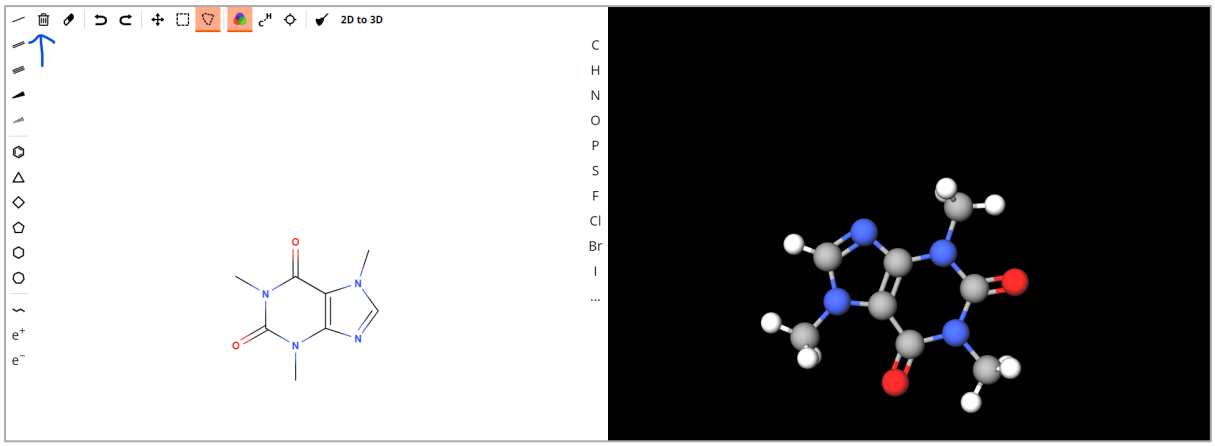
MolView Website

Access MolView via: www.molview.org

Click 'Close' to access the program.



Clear the screen by selecting the trash can in the upper left corner.

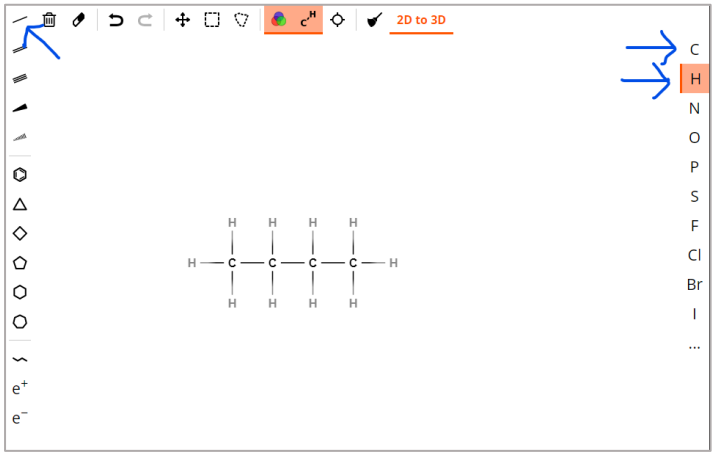


Using the DRAW function

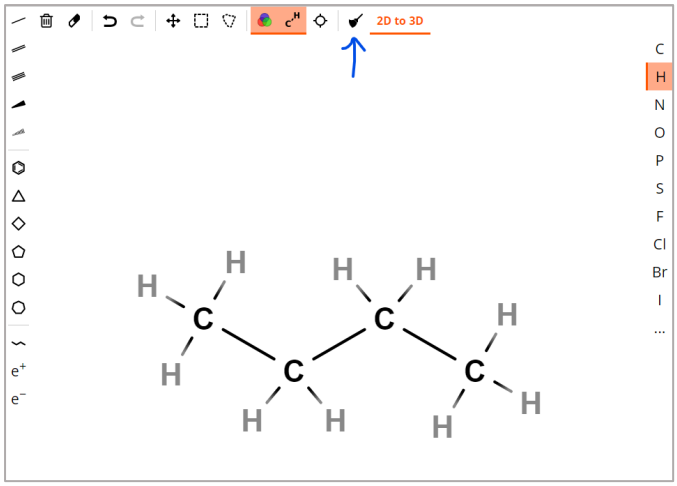
1. **Construct a *butane* molecule (C_4H_{10}; $CH_3CH_2CH_2CH_3$) and use Molview to calculate C-C atomic distance and bond angles.**

a. Use the single bond tool on the top left to draw out the backbone of your molecule. *If you make a mistake you can erase it using the eraser tool (next to the trash can).*

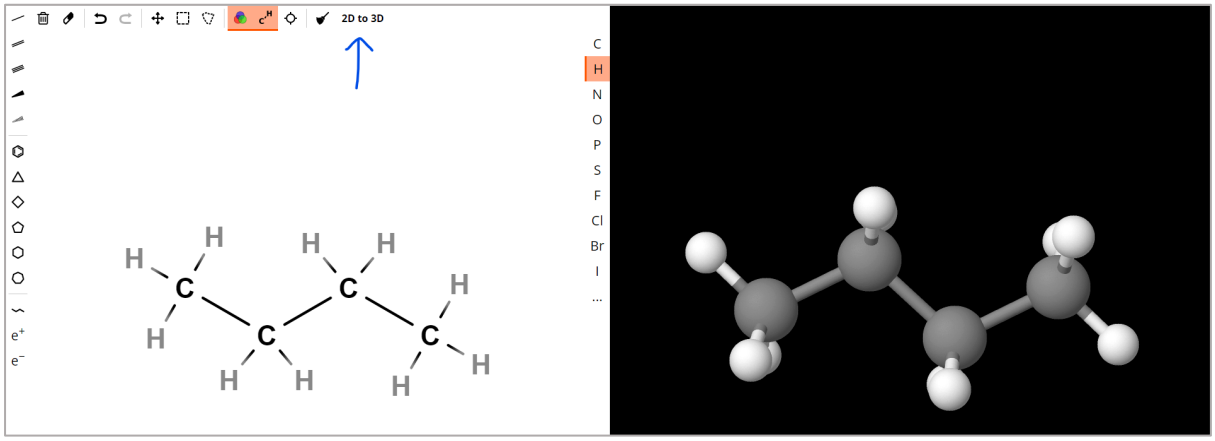
b. Use the atom tools on the right to correctly allocate all atoms as carbons or hydrogens.



c. Clean up the structure by using the broom tool. *Note this will not fix an incorrect structure, for example, a carbon with 5 bonds will be permitted.*

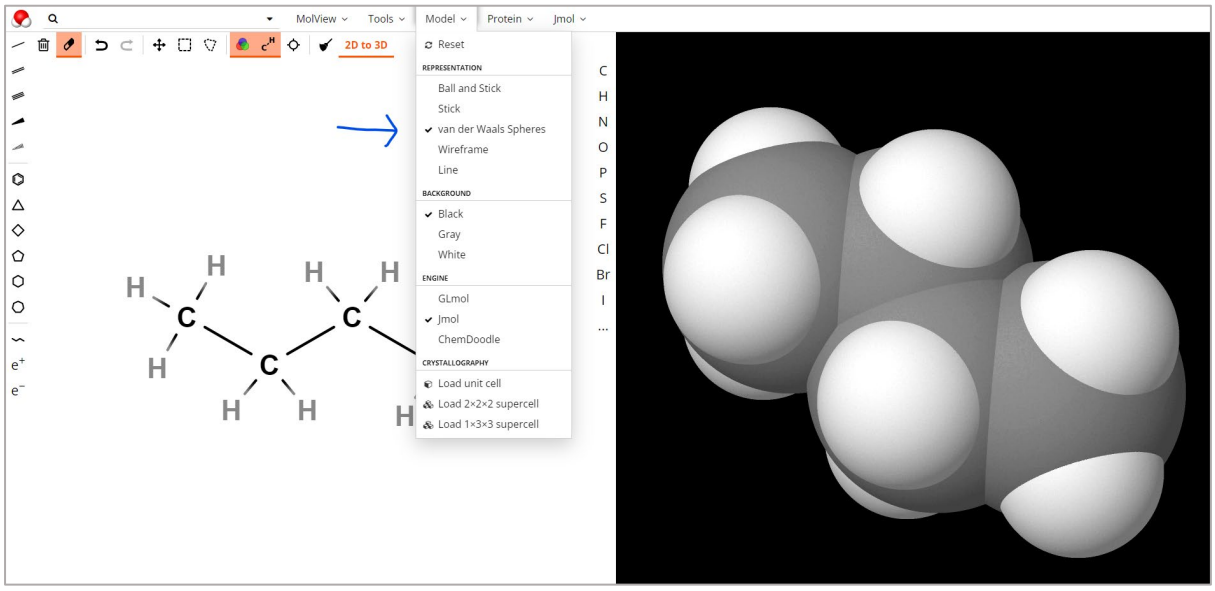


d. Convert the structure from 2D to 3D using the conversion tool.



e. Rotate the 3D view of butane by clicking and dragging with your mouse, zoom in or out on the 3D view of butane using the scroll wheel on your mouse.

f. The current view is a ball and stick model, you can change the model type under ‘model’ to: stick; van der Waals Spheres; Wireframe; or Line. Try each of these now.

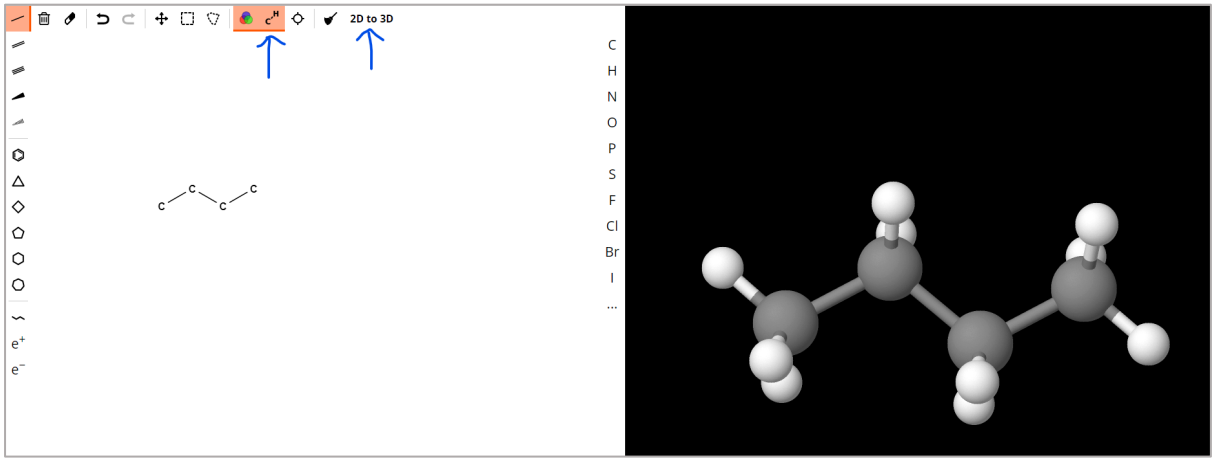


g. Clear the screen

h. Construct butane on the 2D screen again, but this time only draw the 4 carbon backbone (do not add any hydrogens, as shown below)

i. Convert structure from 2D to 3D. The hydrogens will automatically be included in the structure.

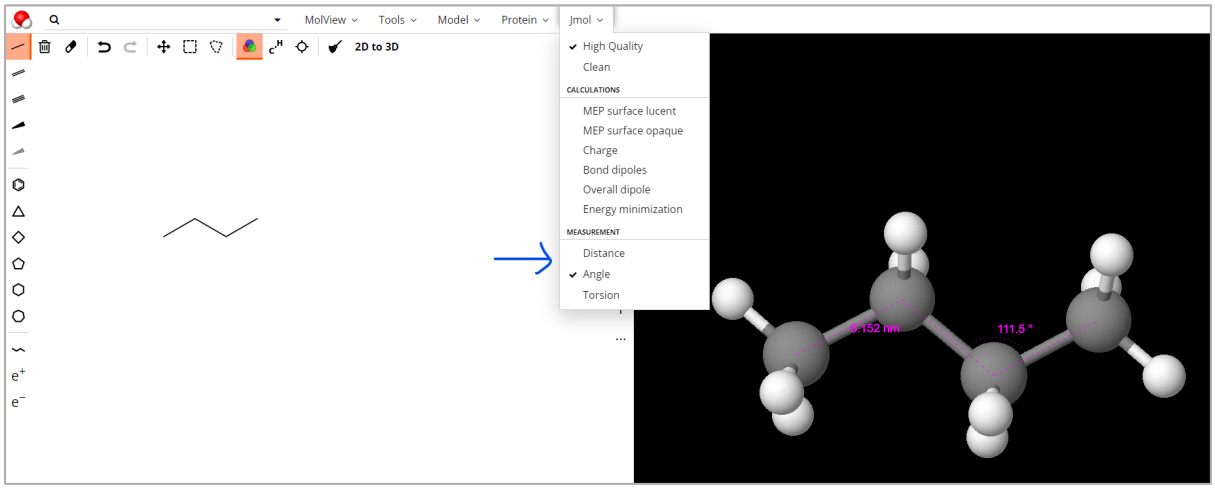
j. On the 2D screen toggle the C-H button on and off to show/hide hydrogens on your 2D structure.



k. You can measure atomic distance and bond angles, before doing this you should perform an energy minimisation (to ensure that the molecule is in its lowest energy conformation). Select 'Energy minimization' under the 'Jmol' tab.

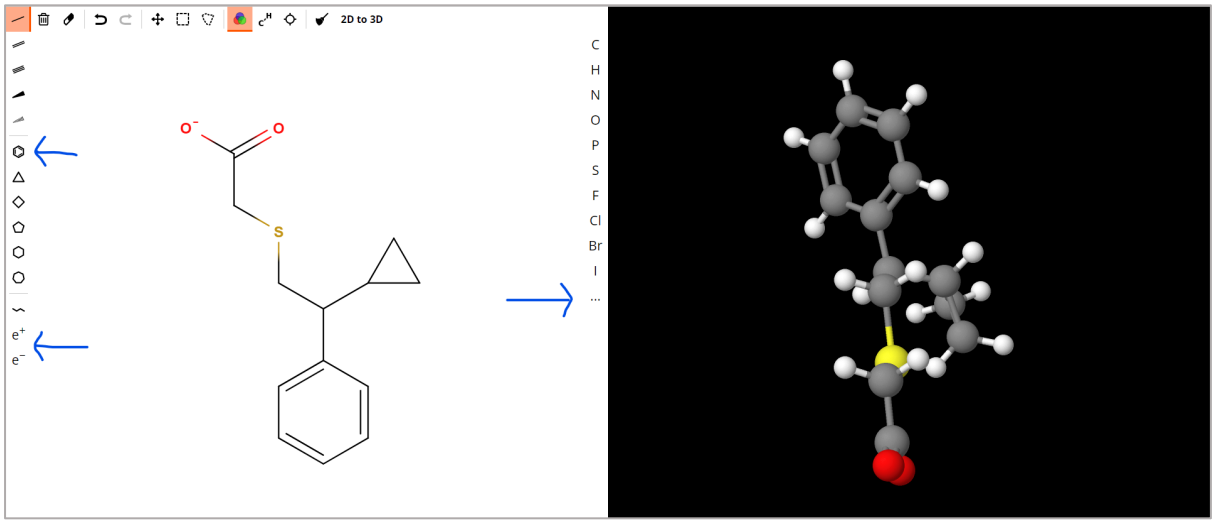
l. Measure the distance between two carbon atoms in butane using the 'Distance' measurement available under 'Jmol'. To show the distance in nm click two adjacent atoms with the distance tool selected.

m. Measure the angle between the carbon atoms of butane using the 'Angle' measurement available under 'Jmol'. To show the angle click three adjacent atoms with the angle tool selected.



2. Construct any molecule you want

a. Take a few minutes to play around with the drawing tools to create a random molecule. Some tools you might want to use include:
   i. Try changing bond types to include double/triple bonds;
   ii. Try adding in cyclic structures/aromatic rings available on the left-hand side;
   iii. Add different atom types, you can access additional elements via the three dots below iodine on the right-hand side;
   iv. Add charges to your molecule using the e^+ and e^- available on the left side.



PART 2: Visualising Dipoles and Polarity

MolView Website

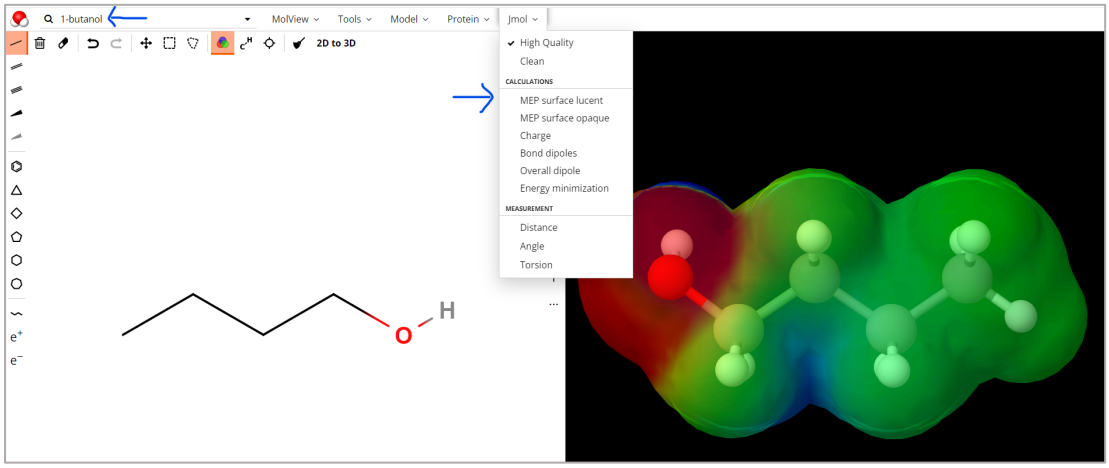
Access MolView via: www.molview.org

Using the NAME function

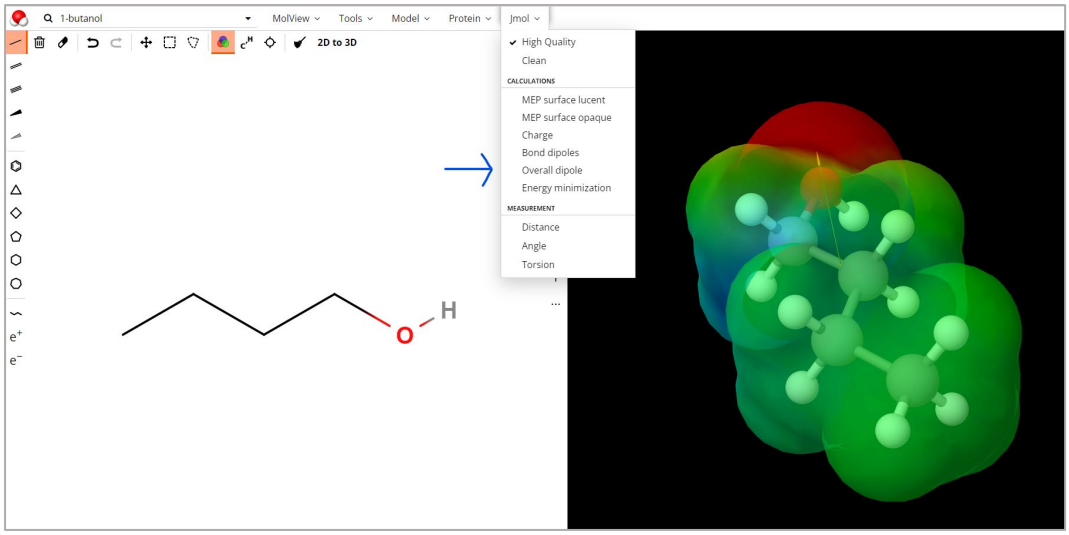
1. **Construct 1-butanol and use Molview to show the dipoles and molecular electrostatic potential for the molecule.**

a. Enter the name '1-butanol' into the search box at the top of the screen. This will automatically produce the named molecule in the 2D and 3D screens. *There is a large database of molecules which will be recognized by name. This can be a useful tool if students need to quickly check they have drawn a structure correctly.*

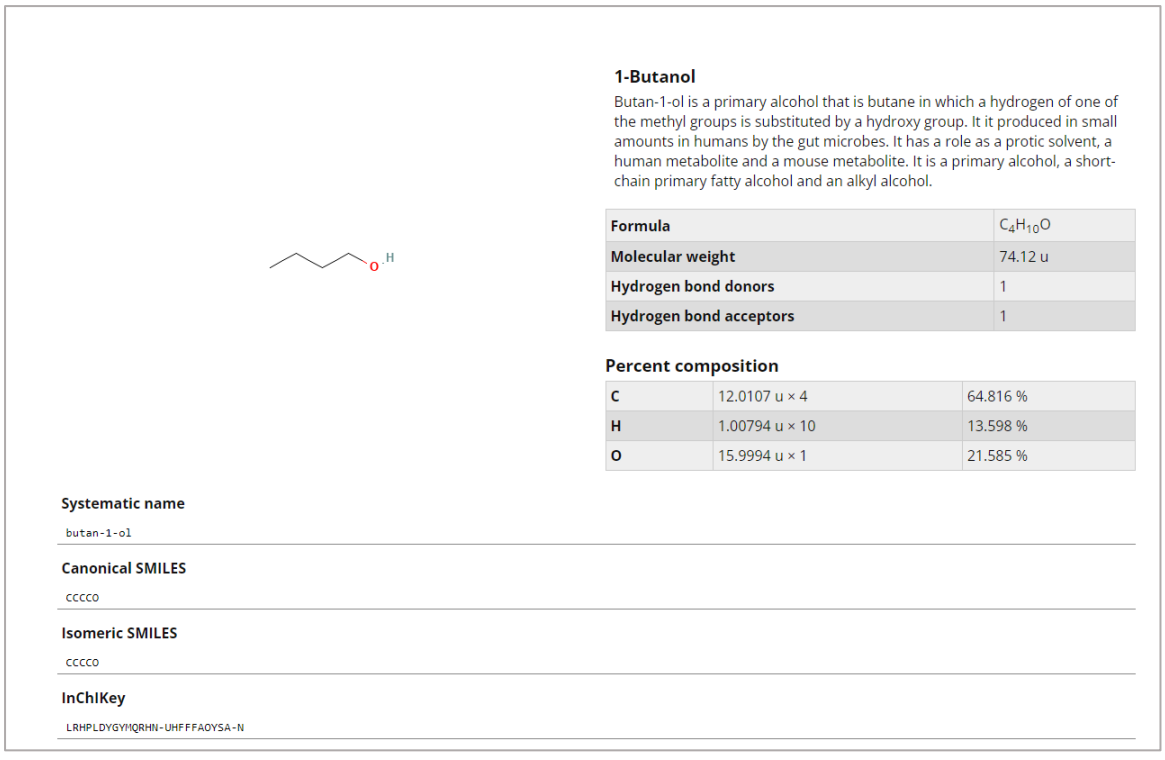
b. Show the molecular electrostatic potential (MEP) by selecting 'MEP surface lucent' available under the 'Jmol' tab. MEP is calculated by probing the molecule with a H^+, regions which attract the H^+ (partial negatively charged regions) are shown in red; regions which repel the H^+ (partial positively charged regions) are shown in blue; regions with no charge (non-polar) are shown in green.



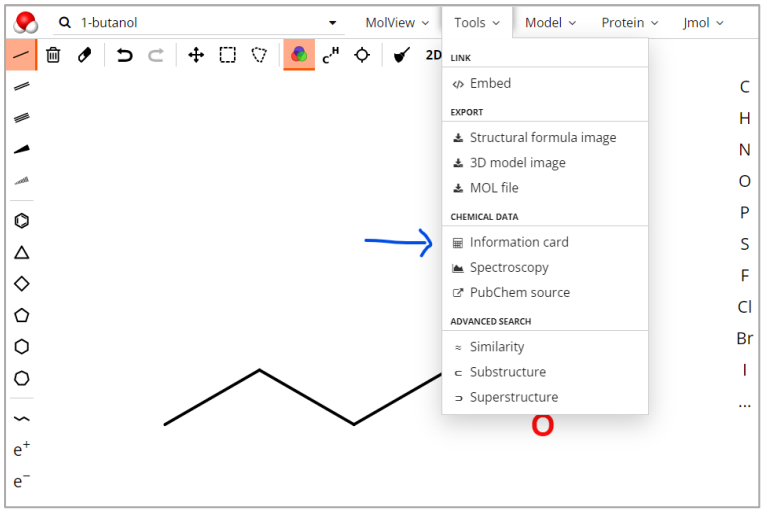
c. Add the molecular dipole on the molecule by selecting 'Overall dipole' under the 'Jmol' tab, this adds an arrow with the arrow head pointing to the region of highest electron density. You can also add 'Charge' and 'Bond Dipoles' using the same tab.



d. Click on the 'Information card' option available under the 'Tools' tab. If the molecule is recognised by the database this will provide information on compound name, formula, molecular weight etc…



e. You can save the 2D structure using 'Structural formula image' and the 3D structure using '3D model image' under the 'Tools' tab.



PART 1 & 2 Additional Resources: CheMagic Website

Access CheMagic via: https://chemagic.org/molecules/amini.html

CheMagic has similar capabilities but it is a little bit less user friendly, but useful if you want to expose students to different web applications. Capabilities include:

- Drawing 2D structures → 3D models
- Name → structure
- Measuring bond length and angles
- Showing dipoles and polarity
- Producing 2D and 3D structures for reports

PART 3: Visualising Complex Organic Molecules

Module 7: Organic Chemistry

POLYMERS

Inquiry question: What are the properties and uses of polymers

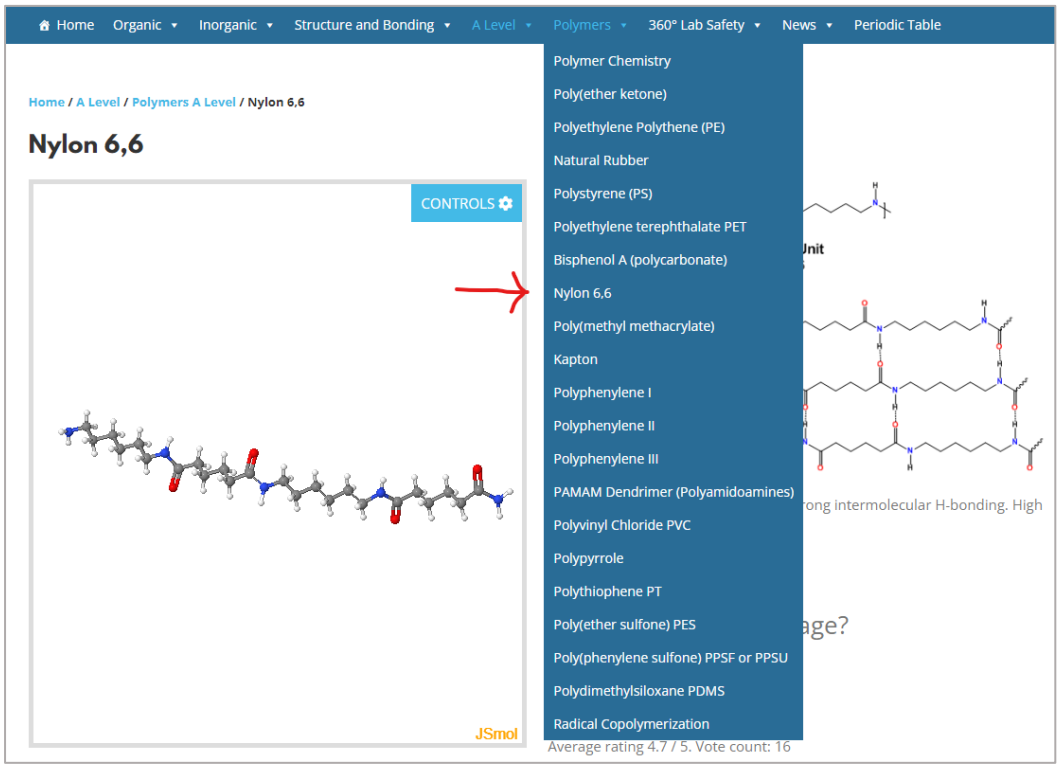
- Model and compare the structure, properties and uses of addition polymers or ethylene and related monomers, for example: polyethylene, polyvinyl chloride, polystyrene, polytetrafluoroethylene.
- Model and compare the structure, properties and uses of condensation polymers, for example: nylon, polyesters.

ChemTube3D Website

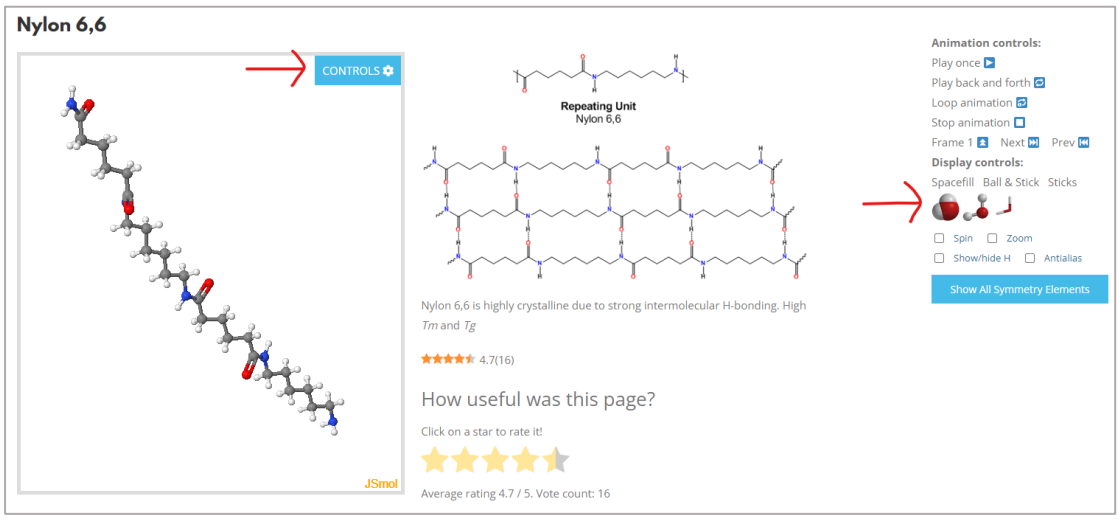
Access ChemTube3D via: www.chemtube3d.com/main-page/

1. Examine the structure of condensation polymer nylon 6,6 and determine its repeating unit

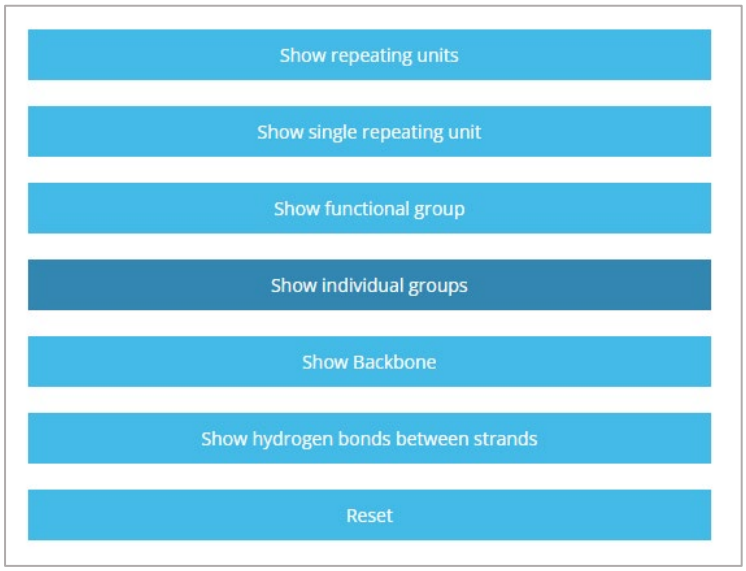
a. Under the 'Polymers' tab select 'Nylon 6,6'. This will show nylon 6,6 in the 3D window. The molecule in the 3D window can be rotated (click and drag mouse) and zoomed in/out (mouse scroll wheel).



b. Change the appearance of the molecule by clicking the ‘Controls’ button in the top right corner and then selecting ‘Space fill’ or ‘Sticks’.



c. Beneath the 3D window are tabs which provide additional information about the polymer structure. Click each of these in turn. These help identify the repeating unit of the polymer, the functional groups and the intermolecular hydrogen bonds.



Part 3 Additional Resources: Molview Website

Access Molview via: www.molview.org

Molview enables you to visualise the 3D structure of proteins, clearly identifying secondary, tertiary and quaternary structure.

PART 4: Visualising Organic Reactions

Model 7: Organic Chemistry

PRODUCTS OF REACTIONS INVOLVING HYDROCARBONS

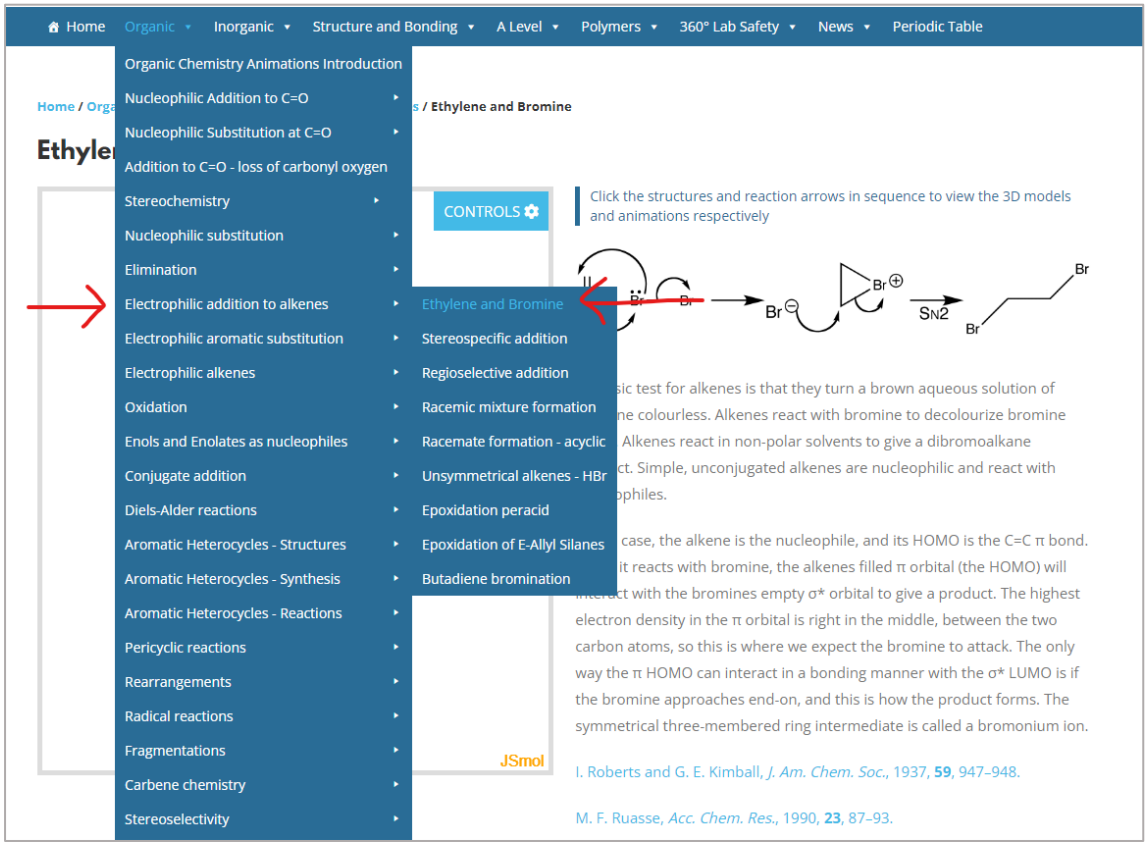
Inquiry question: What are the products of reaction of hydrocarbons and how to they react?

- Investigate, write equations and construct models to represent the reactions of unsaturated hydrocarbons when added to a range of chemicals, including but not limited to: hydrogen, halogens, hydrogen halides and water.

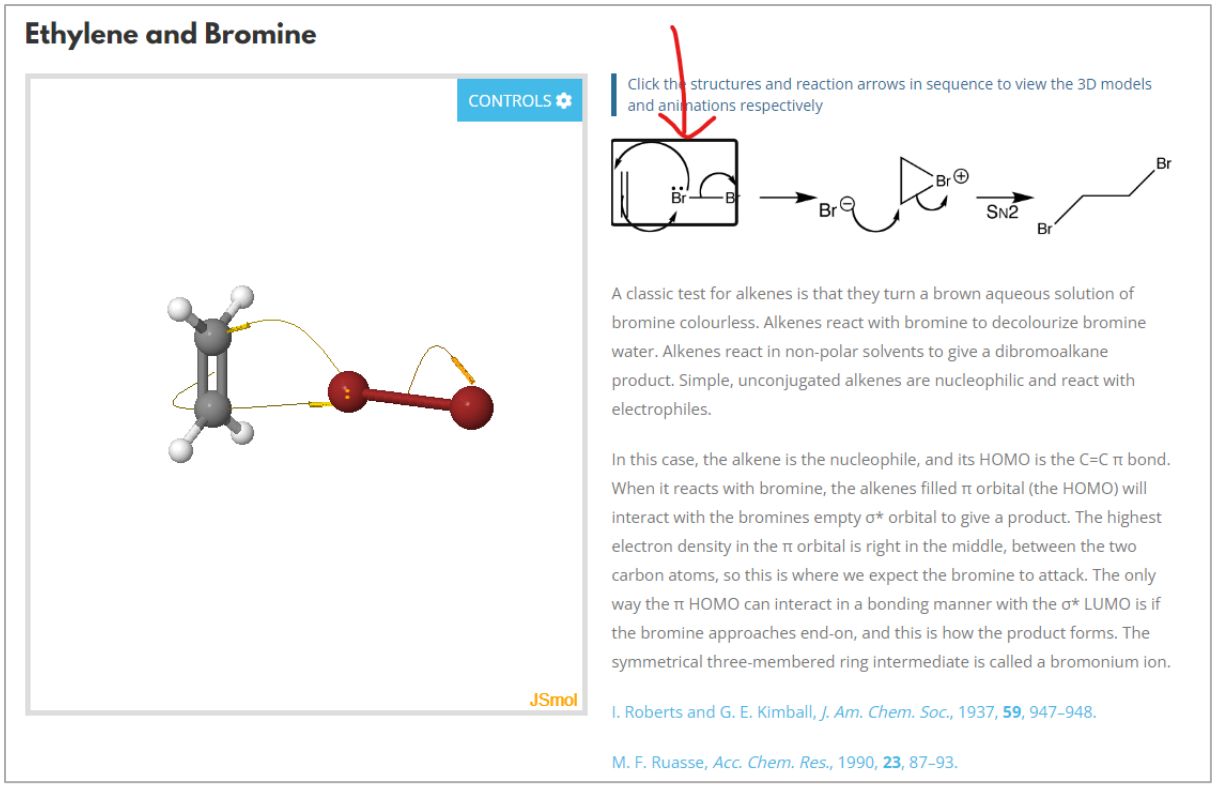
ChemTube3D Website

1. Examine the mechanism for the addition of bromine to an alkene

a. Under the 'Organic' tab select 'Electrophilic addition to alkenes' and then 'Ethylene and Bromine'



b. Clicking on the individual steps of the 2D reaction will display that step in the 3D window with mechanistic arrows. This can be rotated and examined. This allows for a 3D analysis of the mechanism for this reaction with a particular focus on the 3D shape of intermediates in organic chemistry reactions.



2. Examine the mechanism for the addition of bromine to an alkene

a. Under the ‘Organic’ tab select ‘Electrophilic addition to alkenes’ and then ‘Unsymmetrical alkenes – HBr’.