

# Online virtual molecular modelling kits

STANSW Workshop 2022

Presented by Dr Jody Moller

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## PART 1: Visualising Simple Organic Molecules

### Module 7: Organic Chemistry

#### HYDROCARBONS

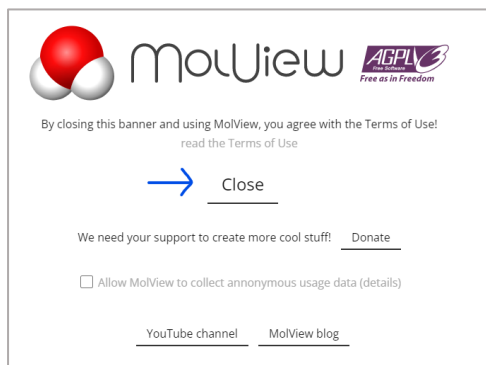
**Inquiry question:** How can hydrocarbons be classified based on their structure and reactivity?

- 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

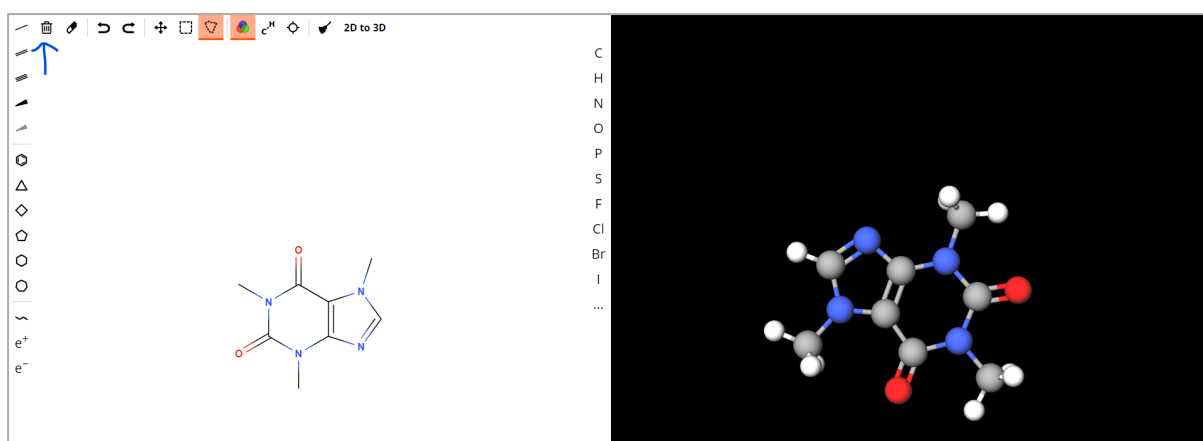
### MolView Website

Access MolView via: [www.molview.org](http://www.molview.org)

Click 'Close' to access the program.



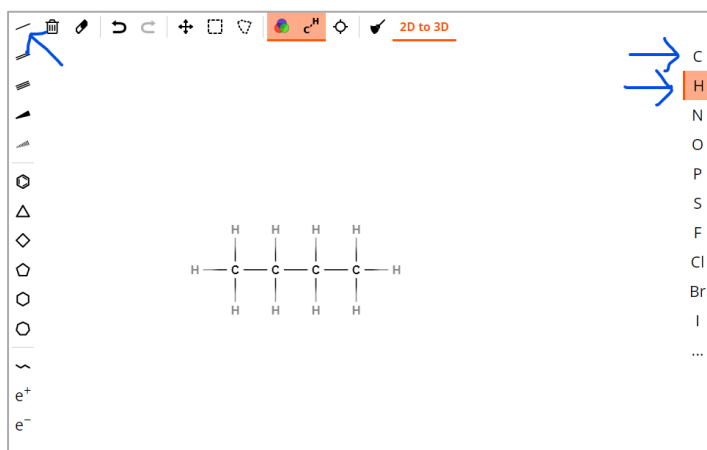
Clear the screen by selecting the trash can in the upper left corner.



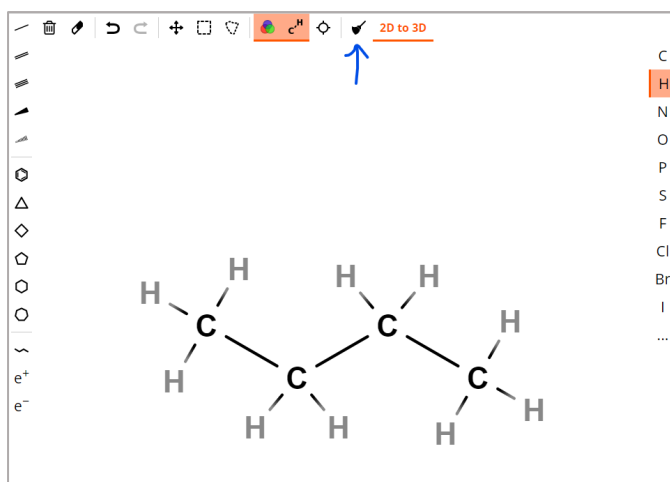
## Using the DRAW function

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.

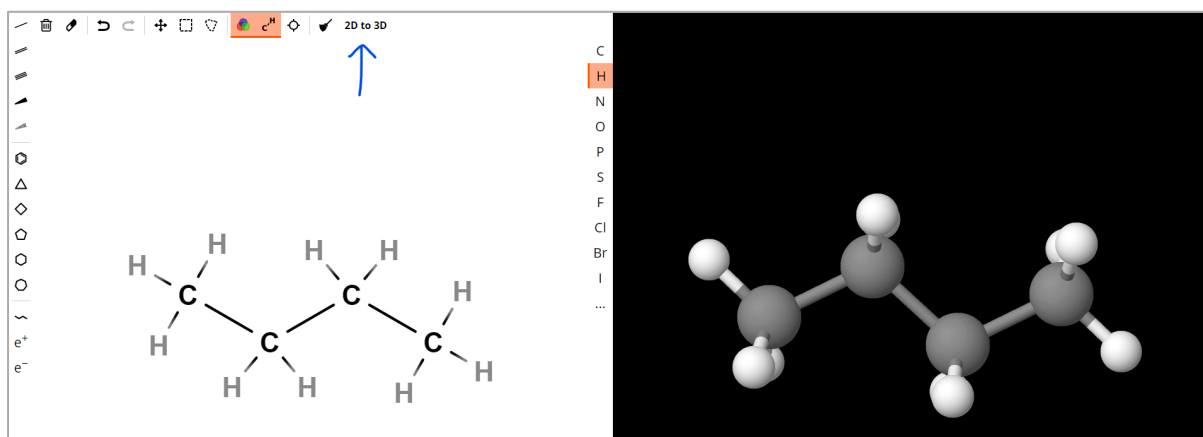
- Use the single bond tool on the top left to draw out the backbone of your molecule. *If you make a mistake you can erase it using the eraser tool (next to the trash can).*
- Use the atom tools on the right to correctly allocate all atoms as carbons or hydrogens.



- 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.*

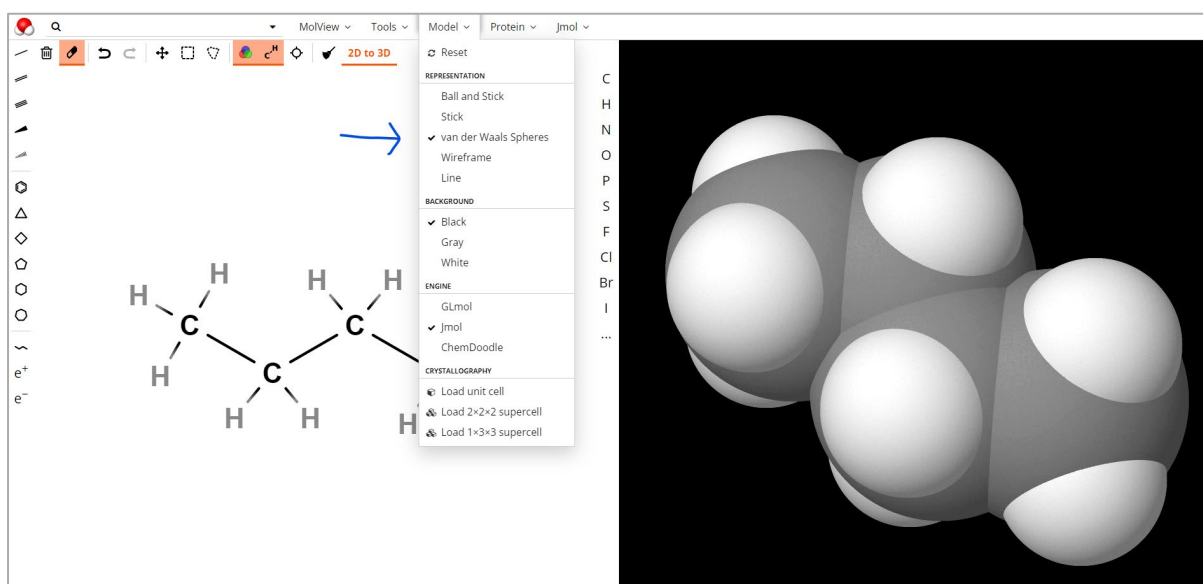


d. Convert the structure from 2D to 3D using the conversion tool.

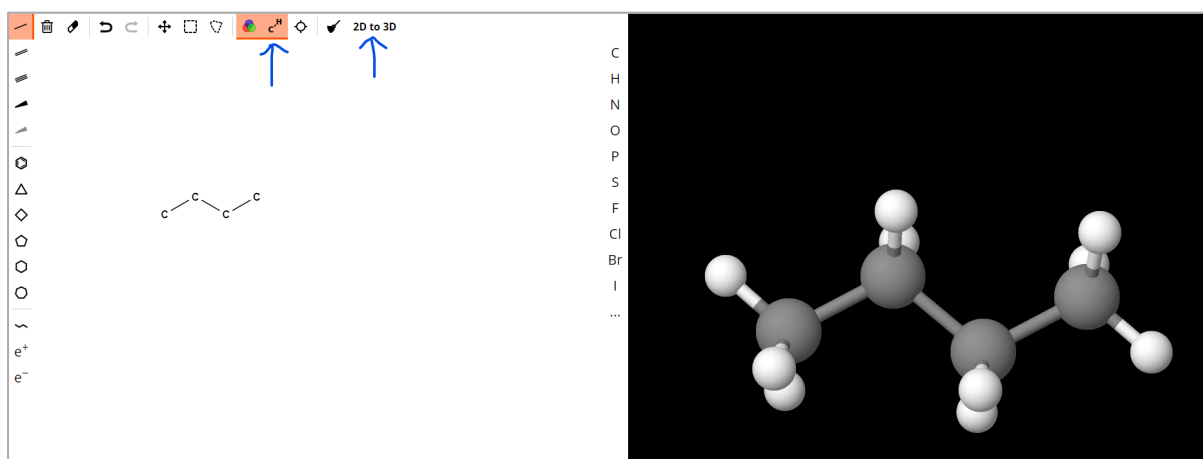


e. Rotate the 3D view of butane by clicking and dragging with your mouse, zoom in or out on the 3D view of butane using the scroll wheel on your mouse.

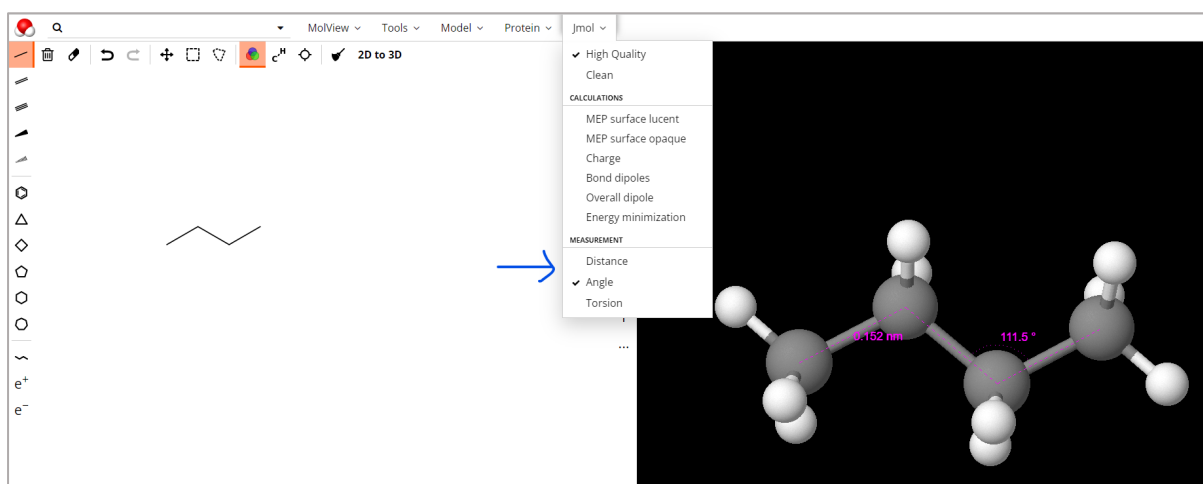
f. The current view is a ball and stick model, you can change the model type under 'model' to: stick; van der Waals Spheres; Wireframe; or Line. Try each of these now.



- 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.

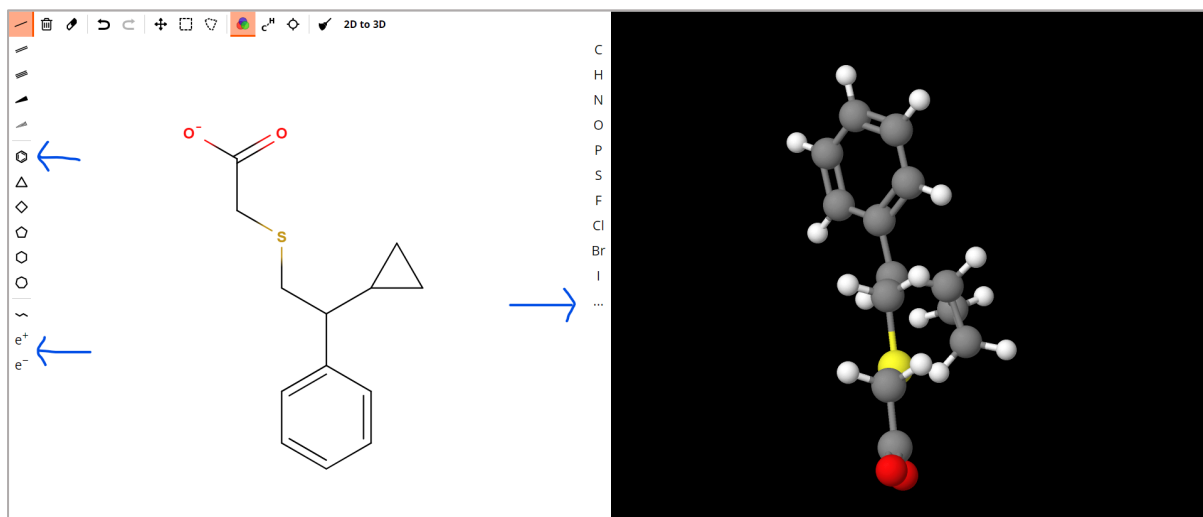


- k. You can measure atomic distance and bond angles, before doing this you should perform an energy minimisation (to ensure that the molecule is in its lowest energy conformation). Select 'Energy minimization' under the 'Jmol' tab.
- l. Measure the distance between two carbon atoms in butane using the '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:
- Try changing bond types to include double/triple bonds;
  - Try adding in cyclic structures/aromatic rings available on the left-hand side;
  - Add different atom types, you can access additional elements via the three dots below iodine on the right-hand side;
  - Add charges to your molecule using the  $e^+$  and  $e^-$  available on the left side.



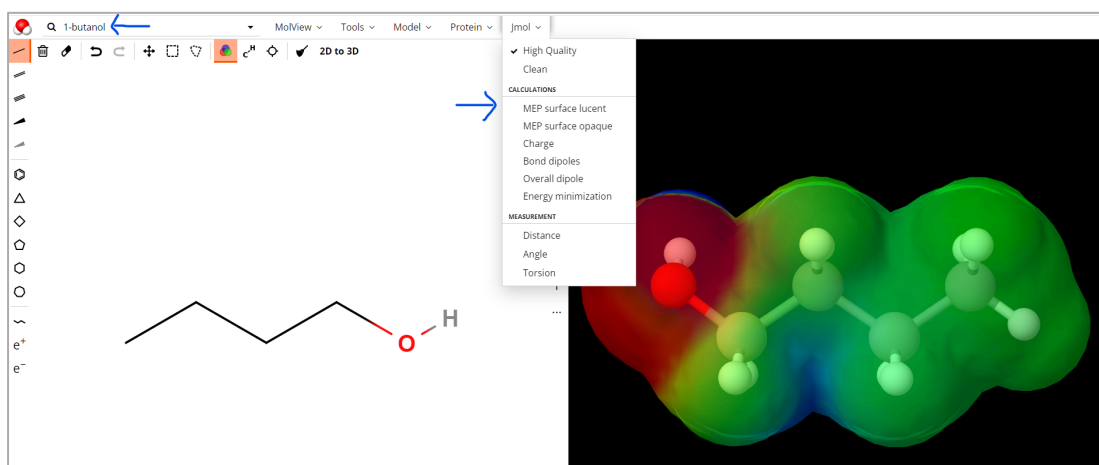
## PART 2: Visualising Dipoles and Polarity

### MolView Website

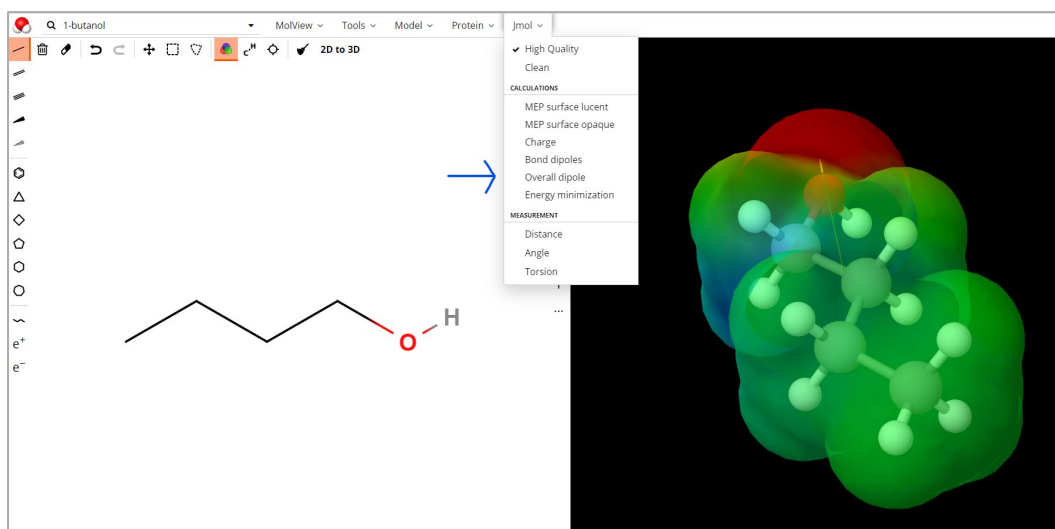
Access MolView via: [www.molview.org](http://www.molview.org)

### 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...



**1-Butanol**

Butan-1-ol is a primary alcohol that is butane in which a hydrogen of one of the methyl groups is substituted by a hydroxy group. It is produced in small amounts in humans by the gut microbes. It has a role as a protic solvent, a human metabolite and a mouse metabolite. It is a primary alcohol, a short-chain primary fatty alcohol and an alkyl alcohol.

<b>Formula</b>	C <sub>4</sub> H <sub>10</sub> O	
<b>Molecular weight</b>	74.12 u	
<b>Hydrogen bond donors</b>	1	
<b>Hydrogen bond acceptors</b>	1	

**Percent composition**

<b>C</b>	12.0107 u × 4	64.816 %
<b>H</b>	1.00794 u × 10	13.598 %
<b>O</b>	15.9994 u × 1	21.585 %

**Systematic name**

butan-1-ol

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**Canonical SMILES**

CCCCO

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**Isomeric SMILES**

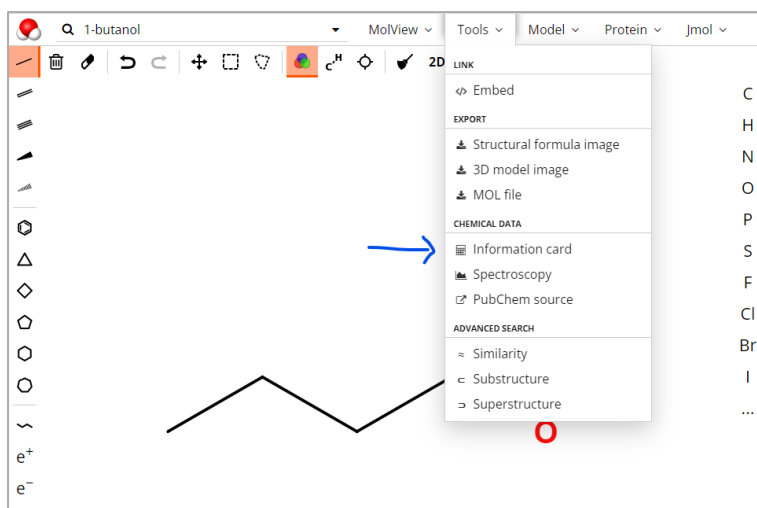
CCCCO

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**InChIKey**

LRHPLDYGYYIQRHJ-UHFFFAOYSA-N

- 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

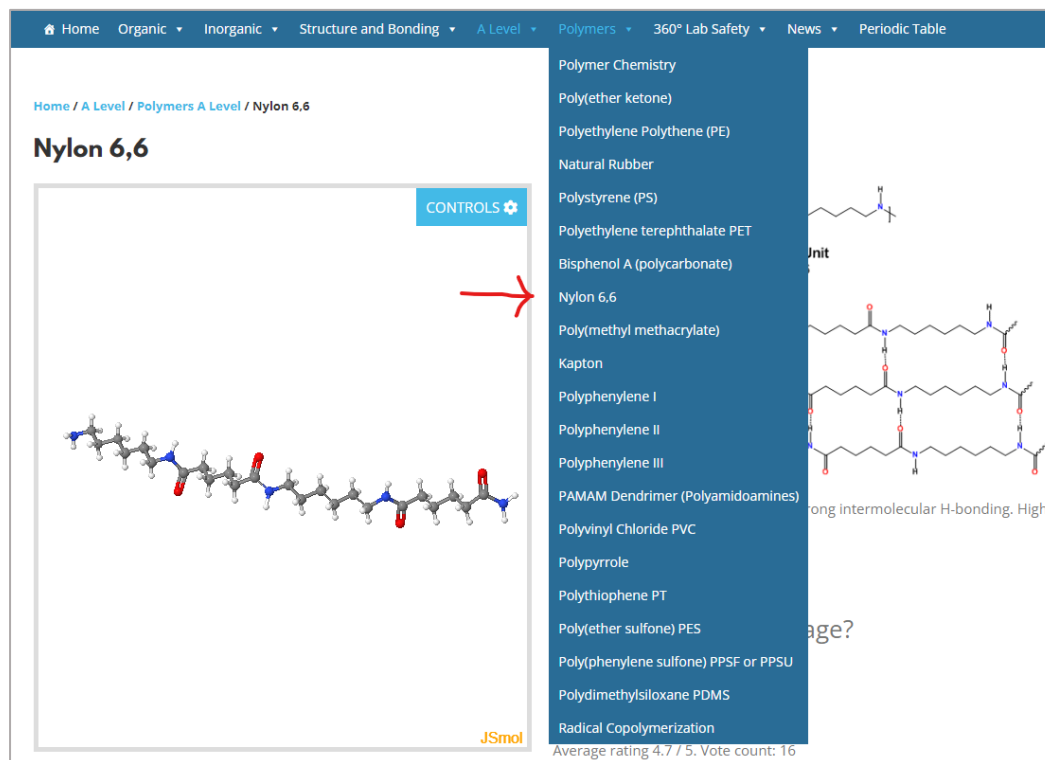
- Model and compare the structure, properties and uses of addition polymers or ethylene and related monomers, for example: polyethylene, polyvinyl chloride, polystyrene, polytetrafluoroethylene.
- Model and compare the structure, properties and uses of condensation polymers, for example: nylon, polyesters.

#### ChemTube3D Website

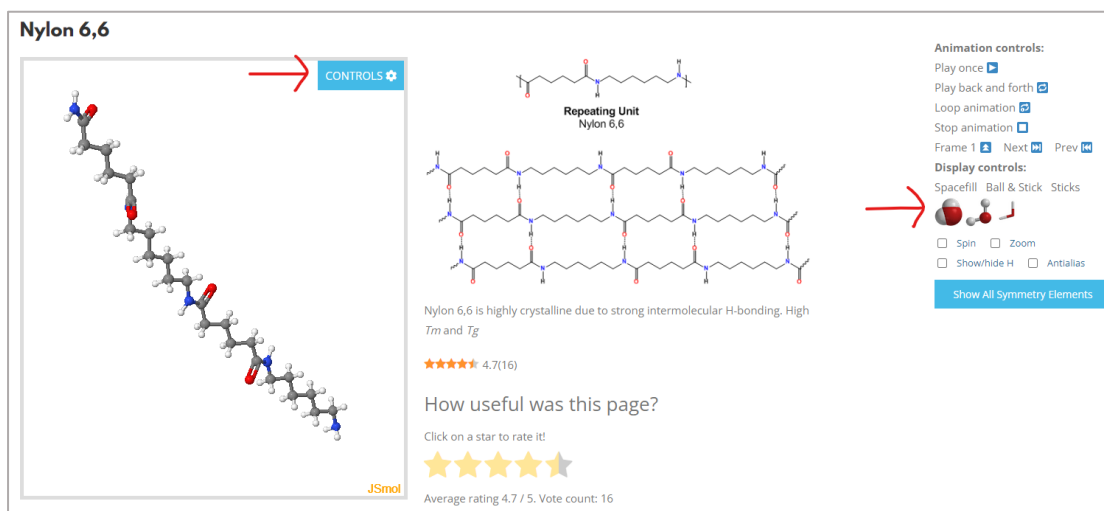
Access ChemTube3D via: [www.chemtube3d.com/main-page/](http://www.chemtube3d.com/main-page/)

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

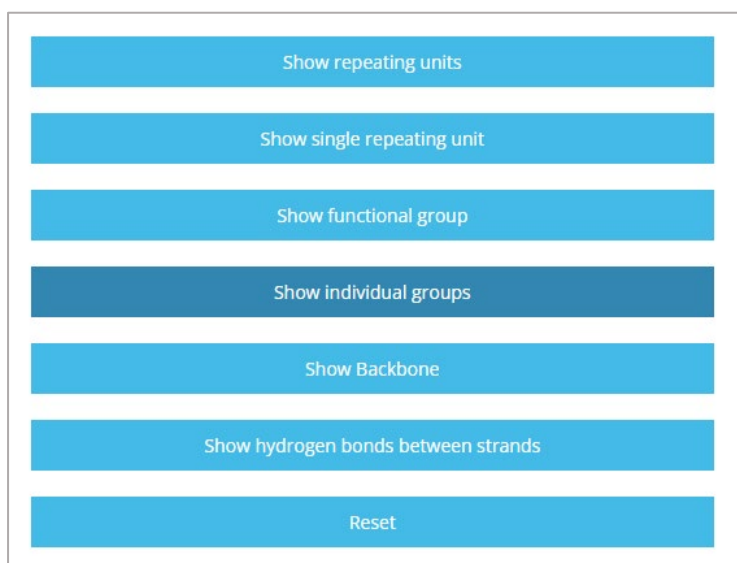
- a. Under the 'Polymers' tab select 'Nylon 6,6'. This will show nylon 6,6 in the 3D window. The molecule in the 3D window can be rotated (click and drag mouse) and zoomed in/out (mouse scroll wheel).



- 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](http://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 do 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

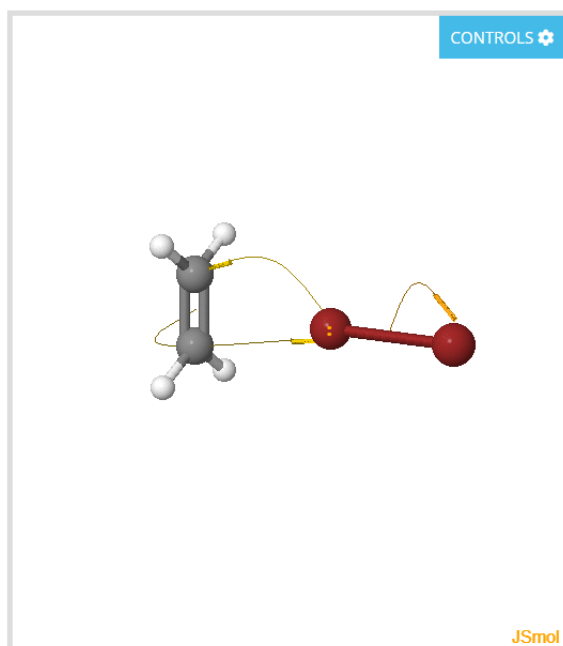
#### 1. Examine the mechanism for the addition of bromine to an alkene

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

The screenshot displays the ChemTube3D website interface. The top navigation bar includes links for Home, Organic, Inorganic, Structure and Bonding, A Level, Polymers, 360° Lab Safety, News, and Periodic Table. A left-hand menu lists various organic chemistry topics, with 'Electrophilic addition to alkenes' highlighted by a red arrow. The main content area shows the 'Ethylene and Bromine' reaction mechanism. It includes a 'CONTROLS' button and a series of chemical structures and arrows illustrating the reaction steps: 1. Ethylene reacts with a bromine molecule (Br-Br). 2. A curved arrow shows the pi electrons of the ethylene double bond attacking one of the bromine atoms. 3. Another curved arrow shows the Br-Br bond breaking, with electrons moving to the other bromine atom. 4. This forms a bromonium ion intermediate (a three-membered ring with a positive charge on the bromine atom) and a bromide ion (Br-). 5. A final step shows the bromide ion attacking the bromonium ion, leading to the formation of 1,2-dibromoethane. Text on the right explains the mechanism: 'The basic test for alkenes is that they turn a brown aqueous solution of bromine colourless. Alkenes react with bromine to decolourize bromine. Alkenes react in non-polar solvents to give a dibromoalkane. Simple, unconjugated alkenes are nucleophilic and react with electrophiles. In this case, the alkene is the nucleophile, and its HOMO is the C=C π bond. It reacts with bromine, the alkenes filled π orbital (the HOMO) will interact with the bromine's empty σ\* orbital to give a product. The highest electron density in the π orbital is right in the middle, between the two carbon atoms, so this is where we expect the bromine to attack. The only way the π HOMO can interact in a bonding manner with the σ\* LUMO is if the bromine approaches end-on, and this is how the product forms. The symmetrical three-membered ring intermediate is called a bromonium ion.' Citations at the bottom include: 'I. Roberts and G. E. Kimball, J. Am. Chem. Soc., 1937, 59, 947-948.' and 'M. F. Ruesse, Acc. Chem. Res., 1990, 23, 87-93.'

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.

## Ethylene and Bromine



Click the structures and reaction arrows in sequence to view the 3D models and animations respectively



A classic test for alkenes is that they turn a brown aqueous solution of bromine colourless. Alkenes react with bromine to decolourize bromine water. Alkenes react in non-polar solvents to give a dibromoalkane product. Simple, unconjugated alkenes are nucleophilic and react with electrophiles.

In this case, the alkene is the nucleophile, and its HOMO is the C=C  $\pi$  bond. When it reacts with bromine, the alkenes filled  $\pi$  orbital (the HOMO) will interact with the bromine's empty  $\sigma^*$  orbital to give a product. The highest electron density in the  $\pi$  orbital is right in the middle, between the two carbon atoms, so this is where we expect the bromine to attack. The only way the  $\pi$  HOMO can interact in a bonding manner with the  $\sigma^*$  LUMO is if the bromine approaches end-on, and this is how the product forms. The symmetrical three-membered ring intermediate is called a bromonium ion.

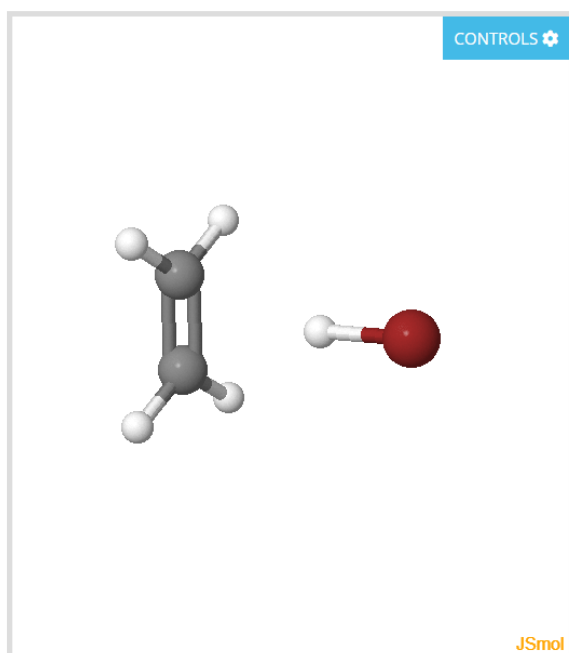
I. Roberts and G. E. Kimball, *J. Am. Chem. Soc.*, 1937, **59**, 947-948.

M. F. Ruesse, *Acc. Chem. Res.*, 1990, **23**, 87-93.

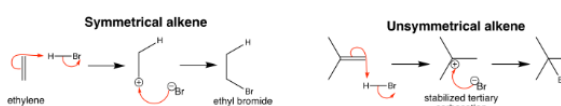
## 2. Examine the mechanism for the addition of bromine to an alkene

- Under the 'Organic' tab select 'Electrophilic addition to alkenes' and then 'Unsymmetrical alkenes – HBr'.

### Electrophilic addition to alkenes – Unsymmetrical alkenes + HBr



Click the structures and reaction arrows in sequence to view the 3D models and animations respectively



In some electrophilic addition reactions, such as those with HBr and an alkene, there is a choice as to which carbon ends up bonded to the H and which the Br. It is important to be able to predict and explain the reactions of unsymmetrical alkenes based on their structures. When HBr reacts with a nucleophile, it is attacked at the hydrogen and loses a bromide ion. Hydrogen cannot form a three-membered cation, so the reaction produces a carbocation. This carbocation then rapidly reacts with the bromide ion, so that overall, the HBr has been added across the alkene.

The bromine atom ends up on the more substituted carbon, which can be understood when you look at the mechanism. Given that a carbocation is formed, the positive charge prefers to reside on the more substituted carbon, giving a more stable tertiary cation as opposed to the alternative much less stable primary cation, which is not formed.

R. C. Kerber, *Found. Chem.*, 2002, **4**, 61-72.