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| Class | Wellington Year 11-12 Chemists |
| Lesson 1 | Skeletal formulae and using computers. |
| Building on | Crude oil is mixture of complex hydrocarbons  Carbon atoms in chains and rings  Fractional distillation  Variation in physical properties  Cracking |
| Learning Objectives | Students should know that a line indicates two carbons bonded together  Hydrogens are implicit  That alkanes are a homologous series  Names of first 10 alkanes  That a computer can be used to manually draw these molecules  That a computer can be used to generate these images and calculate properties |
| Requirements: | Molymods  Jupyter notebook with RDKit, pandas, matplotlib numpy env to work in |
|  | Lessons are an hour long? |
| Starter  5-10 mins | Fractional distillation of crude oil:  Name two fractions – any two from gases petrol, kerosene ,diesel oil, fuel oil, bitumen  What is the difference between them? - Number of carbons. More carbons in one than the other  Which boils first? – the ‘heavier’ fraction  What are they made of? – a mixture of chains and rings of carbons and hydrogens.  Name as many of the the compounds in those fractions as you can. |
| Gases  10 - 15 mins | What are the Gases? – molecular formulae and names  CH4 – Methane  C2H6 – Ethane  C3H8 – Propane  C4H10 – Butane  Make a table in your notes, first column names, then molecular formula, then displayed formula, then two blank columns, then picture of molymod  Fill in first two columns for methane. Build methane in the molymod and take a picture of it. Put it in the last column.  Do the same for the other gases.  How do they differ?  Notice how you take a hydrogen off and add CH3 each time, so effectively adding CH2.  Can you extend this to larger alkanes? Pentane? Hexane?  ~~Use Chem Draw to draw them – can’t use chem draw without skeletal.~~ |
| Structural formulae  5 mins | Methane – CH4 - CH4  Ethane – C2H6 - CH3CH3  Propane – C3H8 - CH3CH2CH3  Butane – C4H10 - CH3CH2CH2CH3  Structural formulae show more of the structure than the molecular formula. The chain is shown as a series of carbon atoms bonded to hydrogens and each other.  Name the first blank column in your table ‘structural formulae’ and add in the structural formula for each of the gases.  Can you extend this to larger alkanes? Pentane? Hexane? |
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| Skeletal Fomulae  5 mins | To chemists, because these are hydrocarbon moleucles we know the hydrogens are there, they don’t tell us anything about the structure.  So we can be lazy, and draw the molecules without the hydrogens.  We also know that the chain must be made of carbons, so we don’t bother to say that they are carbons, we just draw a line between them.  So being even lazier.  Instead of CH3CH3 we draw a single line.  Instead of CH3CH2Ch3, we draw two lines, joined at an angle to make it clear that there are three carbons and two bonds between them.  The angle is similar to the angle you see in the molymods.  Fill in the table using your pen to sketch the skeletal formulae |
| Python via jupyter notebook  20 mins | Open the jupyter notebook provided  Jupyter notebooks contain ‘cells’ which can be writing – mark down and code – Python.  You can run them bit by bit.  The first code cell imports the packages so they are ready for us to use.  Run it please.  The second code cell uses the SMILES code for ethane to define the molecule, and shows you the formula it generates.  The SMILES string for ethane is ‘CC’. Can you guess what methane would be? Experiment by changing the ‘CC’ to ‘C’ or ‘CCC’ or even ‘CCO’  The third code block saves this in to a variable. The name is the same as the chemical name, to make things easy for you to understand. This is a very good principle when coding.  Note there is no output when you do this. You can get the output by just typing in the name of the variable again, and running the cell (this is the fourth cell).  We can use this package to calculate molecular weights and formulae, these are the fifth and sixth cells.  You can also draw this molecule to an image, this is the seventh code cell.  Repeat this code for methane, propane and butane.  In your table add two columns, one for exact molecular weight, and one for the SMILES string. Fill it in after checking your molecular weight and skeletal formulae are correct.  Try other smiles strings.  Confident programmers can use a for loop as a better way to repeat code, for example to generate smiles strings for all the straight chain alkanes and calculate all their molecular weights |
| Summary  2 mins | We have learned how to understand basic structural formulae and skeletal formulae, and how to use code to generate molecular images and calculate basic properties.  Next: For loops for more molecules. |
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