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| Class | Wellington Year 11-12 Chemists |
| Lesson 3 | Arrays and plotting graphs In matplotlib.  Manually creating database or boiling points and plotting it  London forces/van der waals |
| Building on | Crude oil is mixture of complex hydrocarbons  Carbon atoms in chains and rings  Fractional distillation  Variation in physical properties  Cracking  Skeletal formulae and using computers.  smiles strings |
| Last lesson | Students should know that a line indicates two carbons bonded together  Hydrogens are implicit  That alkanes are a homologous series  Names of first 4 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 |
| Learning objectives | Understand that an array should have only one data type in it, while a list can have any number of types  Lists can be manipulated using a for loop, numpy arrays can be manipulated directly  Understand the trend in bp for the straight chain alkanes |
| Requirements: | Jupyter notebook with RDKit, pandas, matplotlib numpy env to work in |
|  | Lessons are an hour long? |
| Starter  5-10 mins | What is the smiles string for Propane?  Prop = ‘CCC’  How would you change this string using Python to the one for hexane?  Concatenate ‘CCC’ or do prop = prop+prop or prop\*2  What does this code return?  for num in range(4):  print(num\*\*2)  0  1  4  9  Be careful, range(4) generates 0,1,2,3 |
| Lists and Arrays (10 mins) | A list is a convenient way to store information. However it is not particularly good for handling numbers.  Work through Code blocks 1-7 in the jupyter notebook  Numpy arrays are better designed for this.  Work though code blocks 8-14 |
| Plotting  (5 mins) | To plot graphs we use a library called matplotlib.pyplot  The command ‘plt.plot() plots a set of points, an x array and a y array define the points.  Plt.plot(x\_arr, y\_arr, ‘k’) plots a black line joining all the points  If you don’t specify the colour, the machine will chose one for you.  You can plot a graph of x^2 vs x just using your array  plt.plot(my\_arr, my\_arr\*\*2) plots a graph of your array against your array squared.  Graphs must have titles, use plt.title(“a graph to show..”)  And axes labels, use plt.xlabel(“x”) and plt.ylabel(“y”)  To do x2 we use “$x^2$”  The dollar signs tell the machine to format the text using latex code, this makes the maths easier.  TODO – plot a graph of x vs x^3 - just reuse the code above. |
| Data  (10 mins) | We can plot useful chemical data too. Look up the boiling points of the first 10 straight chain alkanes and plot them. Make sure you label your axes and give the graph an appropriate title. |
| London Forces (15 mins) | What needs to happen for these molecules to boil?   * Intermolecular forces need to be broken   What are these forces?   * Look at the molecules – build a couple of molecules in molymods.(space filling would be better)   What is this actually?   * Mostly electron clouds * Which will start to polarise each other when they come close * This causes an attraction..  London forces: (aka Van de Waals)  1. Instantaneous dipole – induced dipole (aka van der Waals, London Forces)   Everything has it, because everything has electrons.  More electrons = stronger id-id forces.   1. atom has randomly moving electrons      1. at any instant, more will be on one side than another.          1. This makes an instantaneous dipole. 2. This instantaneous dipole will induce a dipole in any neighbouring atoms.          1. Resulting in a weak attraction.             The longer the chain, the more likely these interactions will occur, which makes them stronger when the molecules are longer. |
|  | Which do you think will have the higher boiling points?  Chlorine (Cl2) or Bromine (Br2)  Nitrogen (N2) or Oxygen (O2)  Phosphorous (P4) or Sulphur(S8)  Propane (C3H8) or Octane (C8H18)  Butane(CH3CH2CH2CH3) or 2-methylPropane (CH3CH(CH3)CH3)   |  |  |  | | --- | --- | --- | | Chlorine -34oC | Bromine 59oC | More electrons in Br2 so bigger temporary dipoles so greater attractions | | Nitrogen -196oC | Oxygen -183oC | Slightly more electrons in oxygen so bigger temporary dipoles so greater attractions | | Phosphorous 281oC | Sulphur 445 oC | More electrons and a larger molecule in sulphur makes there be more and stronger intermolecular forces | | Propane -42oC | Octane 126oC | A longer chain means more electrons and more chances for temporary dipoles to induce dipoles in other molecules so stronger London forces | | Butane -1oC | 2 methyl propane -12oC | Same number of electrons but a shorter chain and more branching means temporary dipoles in methyl propane are less likely to induce diploes in other molecules. | |
| Summary  2 mins | We have learned about numpy arrays, how they are better for handling numbers. We have learned how to plot a graph, give it a title and label its axes.  We have seen the trend in boiling points of the straight chain alkanes, and understand this is due to the increasing temporary dipole induced dipole interactions when the chain is longer, as there are more possible points of contact.  We can compare molecules and say will have stronger intermolecular forces of this type. |
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