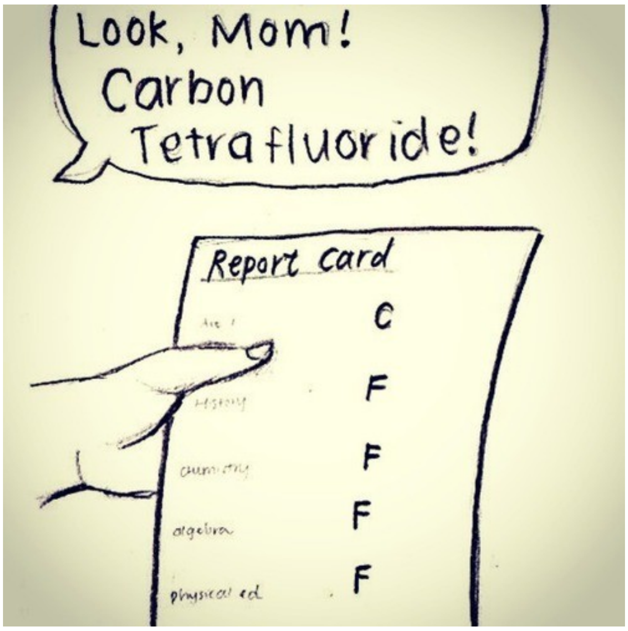
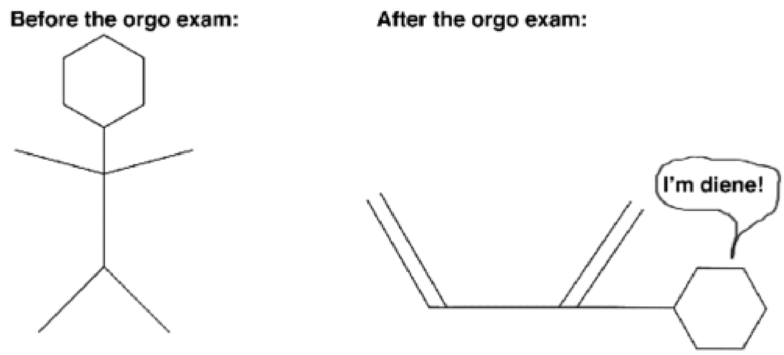
Properties and Structures of Materials

(Organic Chemistry)



(AceOrganicChem.com n.d.)

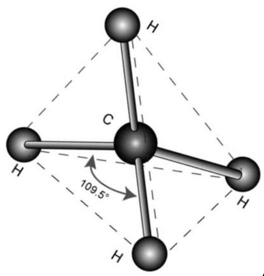


(Arboretictruth 2012)

Week	Outcomes	References and tasks	Tasks
8- 9	• molecular structural formulae (condensed or showing bonds) can be used to show the arrangement of atoms and bonding in covalent molecular substances • IUPAC nomenclature is used to name straight and simple branched alkanes and alkenes from C_1- C_8 • hydrocarbons, including alkanes, alkenes and benzene, have different chemical properties that are determined by the nature of the bonding within the molecules	Lucarelli Set 20, q 1-7 Lucarelli Set 20, q 11-12 Lucarelli Set 20, q 8-10, 13-18	
T1 w10- T2 w1	• alkanes, alkenes and benzene undergo characteristic reactions such as combustion, addition reactions for alkenes and substitution reactions for alkanes and benzene	Lucarelli Set 21, q 1-8	STAWA Investigation 46 pg 108: Reactivity of hydrocarbons Task 5: Test- Properties and Structure of Materials: Organic Chemistry (T2: Week 1) Task 6: Practical test- Post laboratory test 1 (T2: Week 2)

Bonding in Organic Compounds

In organic compounds, carbon is covalently bonded to other non-metals. Carbon has four valence electrons needing four electrons to achieve a stable octet and so forms four covalent bonds. These bonds can be single, double or triple. For example, the "simplest" organic compound is methane (CH_4).



(NA, 2009)

The carbon atom shares one each of its valence electrons with a hydrogen atom. The molecule is actually tetrahedral in shape so as to minimise the repulsion between the four single C-H bonds.

Hydrocarbons are molecular compounds containing the elements hydrogen and carbon. They are classified into various families of compounds based on structural similarities. We will study the families of:

- Alkanes
- Alkenes
- Cycloalkanes
- Cycloalkenes
- Benzene based compounds (aromatics)

Nomenclature (Naming)

1. Find the longest continuous carbon chain. Choose the stem name based on the number of carbon atoms in the longest continuous carbon chain.

Number of Carbons	Stem Name
One	meth-
Two	eth-
Three	prop-
Four	but-
Five	pent-
Six	hex-
Seven	hept-
Eight	oct-
Nine	non-
Ten	dec-

2. Number the carbon atoms sequentially so that the principle functional group has the lowest number.
   The order of priority of the principle functional groups is (from highest to lowest): alkene; halogen then alkyl groups.

   For example: $CH_3CH_2CH{=}CHCH_3$ pent-2-ene

3. If there is a substituted group (eg a halogen), number the carbons from the end which gives the lowest number to the substituted group.

For example: $CH_3CH_2CHCH_3$ 2-chlorobutane

$\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad$ |

$\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad Cl$

4. If there is an alkyl group (other carbon atoms not part of the main chain – also called a branch), name this using the stem name for the number of carbons and use the suffix -yl. Put a number in front to indicate which carbon it comes from then write the stem name.

For example: $-CH_3$ methyl-

$-CH_2CH_3$ ethyl-

$CH_3CH_2CH_2CHCH_2CH_3$ 3-ethylhexane

|

CH_2

|

CH_3

$CH_2CHCH{=}CHCH_3$ 4-methylpent-2-ene

|

CH_3

5. If there is more than one of a substituted group, write the numbers to indicate which carbon they come off, then follow with the prefix di, tri, tetra, penta, etc, then the branch name and -yl. Always finish with the straight chain name.

For example: $CH_3CHCH_2CHCH_2CH_3$

| |

CH_3 CH_3 2,4-dimethhylhexane

6. Note that numbers are separated from words by hyphens and numbers are separated from each other by commas. There should be no spaces or capital letters in the name at all (unless it is the beginning of a sentence).

7. If there are different types of alkyl groups in the same chain, again use numbers, and put the alkyl groups in alphabetical order according to the stem name (note: you disregard the numerical prefix when alphabetizing).

For example: $CH_3CH{-}CH{-}CH\ CH_2CH_3$

| | |

CH_3 CH_3 CH_2

|

CH_3 4-ethyl-2,3-dimethylhexane

8. there are substituted halogens, the same rules apply as for alkyl groups, but use fluoro-, chloro-, bromo- and/or iodo-. Again, substituted groups are named alphabetically.

For example: $CH_3CH_2CH_2CHCHCH_3$

Cl F 3-chloro-2-fluorohexane

9. If there are alkyl groups and substituted halogens, name the halogens before the alkyl groups. If the lowest numbers occur by counting from either end, number so the halogen gets the lowest number. In the case of a tie between two halogens, the first alphabetically gets the lowest number.

For example: $CH_3CH-CH-CH-CHCH_3$

CH_3 CH_3 Cl Cl 2,3-dichloro-4,5-dimethylhexane

10. If there is only one option for a substituted halogen or alkyl groups, do not use numbers.

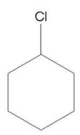
For example: CH_3CHCH_3

CH_3 methylpropane

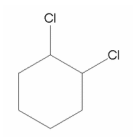
CH_3CH_2Cl chloroethane

Cycloalkanes

1. The name begins with the prefix cyclo- to distinguish it from straight chain aliphatics.
2. Note the shorthand way of drawing rings, where each corner represents a carbon. It is assumed that the remaining bonds are between the carbon and hydrogen atoms.
3. If there is one substituted group, no numbering is required. If there is more than one, numbering is required.



Chlorocyclohexane



1,2-dichlorocyclohexane

Cycloalkenes

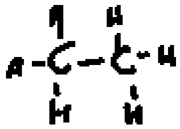
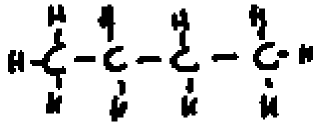
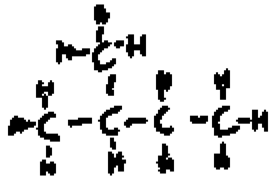
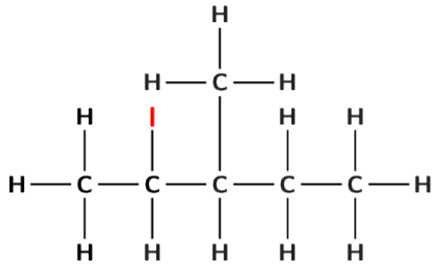
1. Cycloalkenes are named similar to the cycloalkanes (ie add the prefix cyclo-) and the double bond is given the lowest number position.

Benzene

1. Benzene and its derivatives are named similar to cyclic hydrocarbons, but ending with the suffix –benzene.

Alkanes

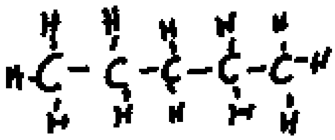
Alkanes are **saturated**, they contain only **single bonds** between carbon atoms. C_nH_{2n+2}

Name	Molecular formula	Structural formula	Condensed formula
Ethane	C_2H_6		CH_3CH_3
Butane	C_4H_{10}		$CH_3CH_2CH_2CH_3$
Methylbutane	C_5H_{12}		$CH_3CH(CH_3)CH_2CH_3$
2-iodo-3-methylpentane	$C_6H_{13}I$		$CH_3CHICH(CH_3)CH_2CH_3$

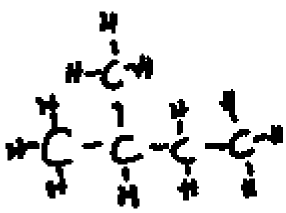
Alkanes: Structural isomerism

Structural isomers are compounds having the same molecular formula but different structural formula.

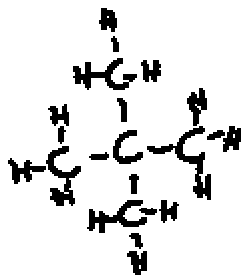
Draw the three structural isomers of C_5H_{12}. Name them and write their condensed formula.



Pentane



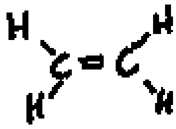
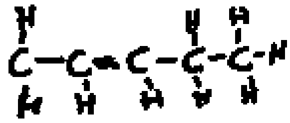
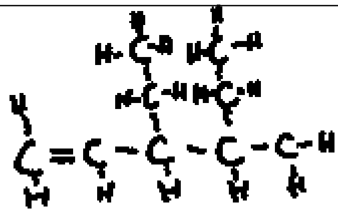
Methylbutane



Dimethylpropane

Alkenes

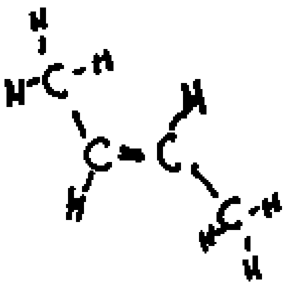
Alkenes contain a **double bond** between carbon atoms and so are **unsaturated**. C_nH_{2n}

Name	Molecular formula	Structural formula	Condensed formula
Ethene	C_2H_4		CH_2CH_2
Pent-2-ene	C_5H_{10}		$CH_3CH_2CHCHCH_3$
3,4-diethylhex-1-ene	$C_{10}H_{20}$		$CH_2CHCH(CH_2CH_3)CH(CH_2CH_3)$[illegible]

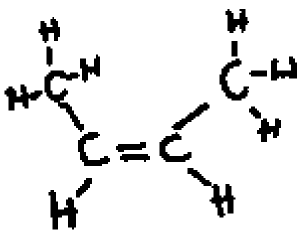
Alkenes: Geometric (cis-trans) isomerism

Geometric isomers have the same molecular and structural formula but a different geometry. The different geometry is a result of the inability of double bonded carbon atoms to rotate along the axis of their double bond.

Draw the **cis** and **trans** isomers of but-2-ene.

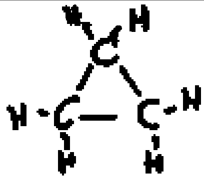
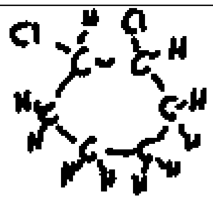
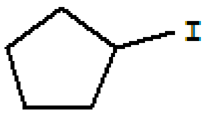


trans but-2-ene

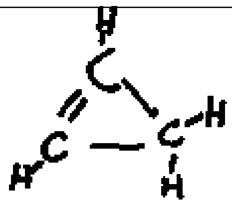
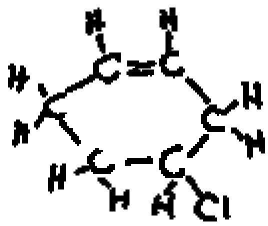
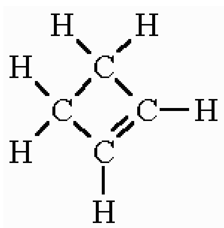


cis but-2-ene

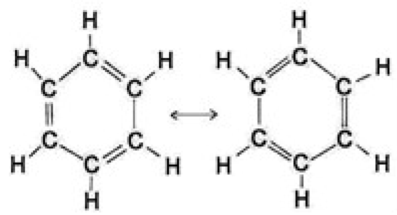
Cycloalkanes

Name	Molecular formula	Structural formula	Condensed formula
cyclopropane	C_3H_6		$CH_2CH_2CH_2$
1,2-dichlorocyclohexane	$C_6H_{10}Cl_2$		$CHClCHClCH_2CH_2CH_2CH_2$
iodocyclopentane	C_5H_9I		$CHICH_2CH_2CH_2CH_2$

Cycloalkenes

Name	Molecular formula	Structural formula	Condensed formula
cyclopropene	C_3H_4		$CHCHCH_2$
4-chlorocyclohexene	C_6H_9Cl		$CHCHCH_2CHClCH_2CH_2$
cyclobutene	C_4H_6		CH_2CH_2CHCH

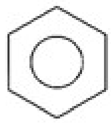
Benzene compounds- aromatics



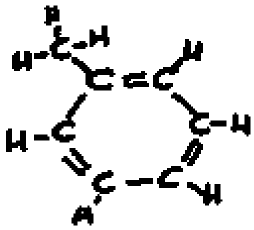
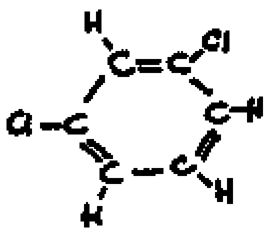
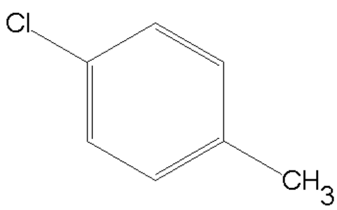
These are the hydrocarbons containing the benzene ring.

The benzene ring has the formula C_6H_6 and is particularly stable.

Due to the arrangement of its electrons, the benzene ring is represented as follows:



Benzene
C_6H_6

Name	Molecular formula	Structural formula	Condensed structural formula
methylbenzene	C_7H_8		$C(CH_3)(CH)_5$
1,3-dichlorobenzene	$C_6H_4Cl_2$		$(CH)_3CClCHCCl$
1-chloro-4-methylbenzene	C_7H_7Cl		$CClCHCH(CH_3)CHCH$

Physical Properties of Hydrocarbons

Melting and Boiling Points

For hydrocarbons of **similar size/ chain length**, the melting point and boiling point depends on how close the molecules can get to each other.

- The closer the molecules are, the greater the intermolecular forces and the greater the mp and bp because more energy is required to overcome these forces.
- How close the molecules can get to each other is dependent on their stereochemistry (ie shape).
- Benzenes can get closer than alkanes which can get closer than alkenes.
- Therefore, mp and bp for similar size/ chain length is: benzene>alkane>alkene

For hydrocarbons of **different size**, the longer the chain (more atoms in molecule), the greater the intermolecular forces.

- This means that the larger the molecule, the greater the mp and bp.
- Eg octane has a higher mp and bp than methane

Chemical Properties of Hydrocarbons

1. Addition

As alkenes are unsaturated, they have the capacity to bond to more atoms. They are therefore more reactive than alkanes and readily undergo addition reactions.

Use condensed structural formula to show the addition reactions for:

a) Pent-1-ene + hydrogen
b) Pent-1-ene + fluorine
c) Pent-1-ene + Hydrogen chloride

2. Substitution

Substitution reactions occur when an alkane or benzene is combined with another element. The C-H bond breaks and the hydrogen is substituted with another element which requires one bond, for example a halogen.

The reactions tend to be slow with one substitution at a time and they require UV light as a catalyst.

Use condensed structural formula to show the substitution reactions for:

a) Ethane + bromine (first substitution)
b) Methane + chlorine (complete substitution)
c) Benzene + Cl_2

3. Combustion

Hydrocarbons are excellent fuels. When ignited in excess air (O_2) they produce carbon dioxide and water vapour and also release considerable amounts of heat energy. This is called complete combustion.

Use molecular formula to write balanced chemical equations for the following combustion reactions (assume complete combustion):

a) Methane in air
b) Butane in air

Incomplete combustion will occur if the air (O_2) supply is limited. Carbon monoxide and even soot (solid carbon) can be produced.

Use molecular formula to write balanced chemical equations for the following reactions where incomplete combustion occurs:

a) Methane in limited oxygen
b) Butane in limited oxygen

Bibliography

AceOrganicChem.com n.d.: , (AceOrganicChem.com n.d.),

Arboretictruth 2012: , (Arboretictruth 2012),