Chemistry Notes: Organic Chemistry

10.1.1: Describe the Features of the Homologous Series

Homologous Series – A group of organic compounds that differ from each other only in the number of carbon atoms they contain.

Alkanes are a homologous series where there are only single bonds. Methane, ethane, propane, and butane are all in one homologous series as they differ only by on CH2 group.

Alkanes have the general formula:

 $C\_{n}H\_{2n+1}$

Other homologous series can be described by a similar functional group.

Functional Group – A small group of atoms attached to a carbon compound that gives characteristic properties to a compound.

Methanol, Ethanol, Propanol and Butanol are all alcohols with the general formula:

 $C\_{n}H\_{2n+1}OH$

10.1.2: Predict and Explain the trends in Boiling Points of Members of a Homologous series

Hydrocarbon Skeleton – The part of the molecule containing only carbon and hydrogen.

 The more CH2 the higher the boiling point of a compound. Compounds with larger hydrocarbon skeletons can be liquid add room temp.

Methane has a small hydrocarbon skeleton and is a gas at room temp while Octane has a large hydrocarbon skeleton and is a liquid at room temp.

 The reason for increased boiling points is that the addition of CH2 increases the number of a temporary dipoles thus causing stronger Van Der Waal’s forces as their relative molecular mass increases.

 The increase is not linear. Greater increases in boiling point occur between Methane and Ethane than Hexane and Heptane as the effect of chain length is proportionally greater for smaller molecules.

 Members of the same homologous series have similar chemical properties because they contain the same functional group.

10.1.3: Distinguish Between Empirical, Molecular, and Structural Formulas

Empirical formula – simplest whole number ratio of the atoms a compound contains.

Molecular formula – the actual number of atoms of each type present in the molecule.

The molecular formula can be deduced given the empirical formula and the molar mass. For example:

30 = (mass of CH3)n 🡪 30 = n(12+(1 x 3)) 🡪 n=2

Molecular formula is C2H6

Molecular formula is also limited because the properties of a compound are not determined by just the number of atoms but their orientation.

Structural Formula – A representation of the molecule showing exactly how the atoms are bonded to each other. Full structural formula shows every bond and atom. Condensed structural formula omits bonds where they can be assumed and groups atoms together.

 There is only one possible structure that can be described by this formula.

For example: The structural formula of ethanoic acid is:



While its condensed structural formula is: $CH\_{3}COOH$

Structural formulas most commonly use 90 or 180 degree bonds. This does not represent their true orientation.

A Stereochemical Formula shows the positions of atoms or groups around carbon in three dimensions. (The bond popping out of the page is a solid black wedge, the bond receding is a dotted line, and the flat bond is a solid line).

For example:



Nomenclature:

Step one: Identify the longest carbon chain. Use the corresponding prefix.

-meth : 1 carbon -eth : 2 carbons –prop : 3 carbons –but : 4 carbons –pent : 5 carbons etc.

Step two: Use the functional group as the last part of the name (suffix).

Alkane: -ane, Alkene: -ene, Alcohol: -anol, Aldehyde: -anal, Ketone: -anone, Carboxylic acid: -anoic acid

Step Three: Name side chains or substituent groups as part of the prefix:

CH3- Methyl

Position of substituent groups is shown by a number followed by a dash that corresponds to the numbered carbon at which it is located. The carbon chain is always counted in such a way so as to give the substituent group the lowest possible numbered position.

C2H5- Ethyl

C3H7- Propyl

F – fluoro

Cl- chloro

Br – Bromo

OH – Hydroxy

NH2 – Amino

If there is more than one side chain in a compound, we us the prefixes di-, or tri-, to refer to the number. If there are two of the same side chains on a single carbon, of the same numbers must be used to denote this, assuming that there are other positions available. For example, if you have two chloro side chains on the second carbon of a four carbon chain, the name of the compound would be:

2,2 – dichlorobutane

(the same rule would apply if you have substituent groups on different carbon locations)

1,2-dichlorobutane

If you have different substituent groups on different carbons:

1-chloro-2-methylbutane.

For functional groups, a similar system is used. In an alcohol, the position of the –OH group is denoted as follows

Propan-2-ol

If the functional group can only be in one place, it is not necessary to include a number.

The ester functional group looks like this:



Esters are organic compounds which form organic acids when they react with alcohols. Esters are named with the suffix –oate, which corresponds to the number of R’s covalently bonded directly to the carbon of the ester group.

Aromatic Compounds:

Aromatic Compounds are compounds which contain a benzene ring C6H6. The benzene ring looks like this:


Benzene is a planar molecule in which six carbons share electrons with themselves and with six hydrogen atoms in a symmetrical arrangement. This is called **delocalization** and makes the benzene ring particularly stable.

Derivatives of the benzene ring include TNT (trinitroluene) in which one hydrogen is replaced by a methyl group, and three others are replaced by nitro groups.

10.1.4: Describe structural isomers as compounds with the same molecular formula but different arrangement of atoms.

Structural isomers are compounds that can be represented by the same molecular formula, but have different arrangements of atoms and therefore varying structural formula’s. **Isomers have varying physical and chemical properties.**

An example of a pair of isomers is 2-methylpropane, and butane. Both consist of four carbons, but 2-methylbutane has a branching methyl group, which decreases the boiling point of the compound relative to butane.

An example of a pair of isomers in alkenes is: pent-1-ene, where the double bond is between the first and second carbon, and pent-2-ene, where the double bond is between the 2nd and 3rd carbon.

IB Objectives 10.1.5 – 10.1.11 are omitted.

10.1.12: Identify primary, secondary, and tertiary carbon atoms in alcohols and halogenoalkanes.

A primary carbon is attached to **one functional group**, at least **two hydrogen’s**, and another **one alkyl group**. Molecules that contain primary carbons are called primary molecules.

The carbon connected to OH and ethanol is a primary carbon.

A secondary carbon is one attached to **one functional group**, **one hydrogen atom**, and **two alkyl groups**. Molecules with secondary carbons are considered secondary molecules.

The middle carbon in propan-2-ol is a secondary carbon.

A tertiary carbon is attached to **one functional group**, **three alkyl groups**, and **no hydrogen atoms**.
Molecules with tertiary carbons are called tertiary molecules.

The carbon attached to three methyl groups and one hydroxyl group in 2-methylpropan-2-ol is a tertiary carbon.

10.1.13: Discuss the volatility and solubility in water of compounds containing the functional groups listed in 10.1.9 (alcohol, aldehyde, ketone, carboxylic acid, and halide).

Volatility is the measure of how easily a substance changes into gaseous state. High volatility means low boiling point. The stronger the intermolecular forces, the higher the boiling point.

As the molar mass of organic compounds increases with the successive addition of CH2, the boiling point of the compound rises do to strengthening Van Der Waal’s forces. So for members of the same homologous series, lower members are likely to be gases or liquids at room temperature, while higher members are likely to be solids.

Branched chain molecules have less contact with each other than straight chain isomers and therefore have lower boiling points.

Functional groups effect volatility and solubility in water. Polar groups will develop dipole-dipole attractions between molecules and therefore have a higher boiling point. Groups which are able to form hydrogen bonds will have even stronger forces and will be soluble in water.

In order from least volatile (higher boiling point and strongest intermolecular forces) to most volatile (lowest boiling point and weakest intermolecular forces), functional groups can be ordered as follows:

Carboxylic acid < Alcohol < Ketone < Aldehyde < Halogenoalkane < Alkane

Solubility in Water:

Two Factors:

 Length of carbon chain: Carbon chain is non-polar so will dissolve in water. Therefore, **the longer the carbon chain**, the **less soluble the molecule**.

Alcohols, Aldehydes, Ketones, and Carboxylic acids can all form hydrogen bonds with water.

Halogenoalkanes cannot form hydrogen bonds with water despite their polarity.

When determining which molecule has the lowest boiling point, first ensure that all molecules have a similar molar mass. Remember that the higher the molar mass, the higher the boiling point.

10.2: Alkanes

10.2.1: Explain the low reactivity of alkanes in terms of bond enthalpies and bond polarity.

General Formula is $C\_{n}H\_{2n+2}$

Alkanes are saturated hydrocarbons, meaning that their carbon-carbon bonds are all single.

Alkanes contain only C-C and C-H bonds. These are both strong bonds and will only break when imposed upon by a strong energy source.

C-C and C-H bonds are both non-polar, meaning that they are not broken by the imposition of polar molecules.

These two factors explain why alkanes are not reactive.

10.2.2: Describe, using equations, the complete and incomplete combustion of alkanes

Two reactions involving alkanes:

Combustion:

Combustion of alkanes is highly exothermic. This is mainly because there is a high amount of energy released in the formation of $CO\_{2}$ and $H\_{2}O$.

In the presence of excess oxygen, alkanes will combust to form carbon dioxide and water.

$$C\_{3}H\_{8}+5O\_{2}\rightarrow 3CO\_{2}+4H\_{2}O ∆H=-2220 kJ mol^{-1}$$

When the oxygen supply is limited, the combustion will produce carbon monoxide and water.

 $2C\_{3}H\_{8}+7O\_{2}\rightarrow 6CO+8H\_{2}O$

 When oxygen is extremely limited, the combustion will produce elemental carbon:

 $C\_{3}H\_{8}+2O\_{2}\rightarrow 3C+4H\_{2}O$

10.2.3: Describe, using equations, the reactions of methane and ethane with chlorine and bromine.

Substitution:

The reaction in which an incoming species will replace one of the hydrogen in the alkane.

Halogens can substitute a hydrogen atom when they split into separate free radicals, which have an unpaired electron.

Initiation: $Cl\_{2}\rightarrow Cl^{.}+Cl^{.}$

This step is called hemolytic fission.

The next step is Propagation because the set of reactions both use and produce free radicals, which allow the reaction to continue.

 $Cl^{.}+CH\_{4}\rightarrow CH\_{3}^{.}+HCl$

 $CH\_{3}^{.}+Cl\_{2}\rightarrow CH\_{3}Cl+Cl^{.}$

 $CH\_{3}Cl+Cl^{.}\rightarrow CH\_{2}Cl^{.}+HCl$

 $CH\_{2}Cl^{.}+Cl\_{2}\rightarrow CH\_{2}Cl\_{2}+Cl^{.}$

The final step is termination. The termination step forces radicals to react with each other and combine electrons.

 $Cl^{.}+Cl^{.}\rightarrow Cl\_{2}$

 $CH\_{3}^{.}+Cl^{.}\rightarrow CH\_{3}Cl$

 $CH\_{3}^{.}+CH\_{3}^{.}\rightarrow C\_{2}H\_{6}$

10.3: Alkenes

10.3.1: Describe, using equations, the reactions of alkenes, with hydrogen and halogens.

The general formula for alkenes is: $C\_{n}H\_{2n}$

Alkenes are unsaturated hydrocarbons containing carbon-carbon double bonds.

 The carbon double bond consists of a σ bond and a π bond.

The **double bond is the site of reactivity** for the molecule.

The π bond is weaker than the σ bond and therefore more easily broken. Thus alkenes undergo addition reactions, in which the double bond is broken and the two new reactive carbon sites become open to react with other atoms.

The products of an addition reaction are saturated.

Hydrogen can react with alkenes to form alkanes with a nickel catalyst at about 150 degrees Celsius. When for example, propene reacts with hydrogen, propane is formed. This process is called hydrogenation.

$$CH\_{2}CH\_{2}CH\_{3}+H\_{2}\rightarrow CH\_{3}CH\_{3}CH\_{3}$$

Halogens react with alkenes to produce dihalogeno compounds. These reactions **happen quickly at room temperature**. They are often accompanied by the loss of the halogen’s color.

 One example of a reaction with a halide is:

$$CH\_{3}CHCH\_{2}+Br\_{2}\rightarrow CH\_{3}CHBrCH\_{2}Br$$

 10.3.2: Describe, using equations, the reactions of symmetrical alkenes with hydrogen halides and water.

Reactions with Hydrogen Halides:

 Hydrogen Halides react with alkenes to produce Halogenoalkanes.

These reactions take place rapidly in solution at room temperature. All hydrogen halides can react, but the most reactive will be the one with the weakest bond. In this case, in order of decreasing reactivity, the common hydrogen halides are:

 HI > HBr > HCl > HF

One example of such a reaction is:

 $CH\_{2}CH\_{2}+HCl\rightarrow CH\_{3}CH\_{2}Cl$

Reactions of Alkenes with water:

 The reaction with water is known as **hydration** and **converts the alkene into an alcohol**. In a lab, the catalyst for such reactions is concentrated sulfuric acid.

 The reaction involves a step in which both the H+ and HSO4- ions are added across the double bond.

 After this step, hydrolysis is achieved by adding water and then replacing the HSO4- ion with OH- thus reforming sulfuric acid:

 $CH\_{2}CH\_{2}^{H\_{2}SO\_{4}}\rightarrow CH\_{3}CH\_{2}\left(HSO\_{4}\right)^{H\_{2}O}\rightarrow CH\_{3}CH\_{2}OH+H\_{2}SO\_{4}$

Conditions required: heat with steam and concentrated sulfuric acid as catalyst.

10.3.3: Distinguish between alkenes and alkanes using bromine water:

Using the fact that alkenes readily undergo addition reactions, while alkanes undergo substitution with UV light, it is possible to immerse and alkane and an alkene in respective vessels of bromine water and distinguish between an alkane and an alkene. **The alkenes addition reaction will remove the red-brown color of Bromine, while the alkane will not.**

10.3.4: Outline the Polymerization of alkenes

Because alkenes undergo addition reactions by breaking their double bonds, they can be joined together to produce long chains called polymers. The alkene used in the reaction is a monomer.

Example: Ethene polymerizes to form poly-ethene.

Polymerization reactions are shown as a constant n, multiplied by the original monomer yielding the repeating unit of the polymer in a bracket with the subscript n.

10.3.5: Outline the economic importance of Alkenes:

Alkenes are polymerized to form many types of construction materials, packaging and electrical cables. PVC, or poly vinyl chloride, is achieved through the polymerization of chloroethene and is one of the worlds most important plastics. One disadvantage of its production is that one of its byproducts is dioxin.

Polytetrafluoroethene is also important as it is non-adhesive and comprises many layers of waterproof fabrics.

10.4: Alcohols

10.4.1: Describe, using equations, the complete combustion of alcohols.

The general formula for an alcohol is:

 $C\_{n}H\_{2n+1}OH$

Alcohols have the OH functional group. As this is a polar group, it increases solubility in water.

Combustion:

Alcohols burn in oxygen to produce carbon dioxide and water. The amount of energy released per mole increases as we move up the homologous series (this is mainly due to the increasing amount of carbon dioxide produced).

For example: the burning of methanol is show by the equation below:

$$2CH\_{3}OH+3O\_{2}\rightarrow 2CO\_{2}+4H\_{2}O$$

Here, there is a 1:1 ratio of methanol to carbon dioxide and the heat of reaction is 726.1 kj per mol.

On the other hand, in the combustion of pentanol, where the carbon dioxide-alcohol ratio is 5:1, the heat of reaction is 3330.9 kj per mole.

 $2C\_{5}H\_{11}OH+15O\_{2}\rightarrow 10CO\_{2}+12H\_{2}O$

As with the combustion of hydrocarbons, a limited supply of oxygen will result in the production of carbon monoxide.

10.4.2: Describe, using equations, the oxidation reactions of alcohol.

In oxidation reaction of alcohols, the oxidizing agent oxidizes the carbon atom attached to the OH- group. The most common oxidizing agent is potassium dichromate(VI). When the reaction mixture is heated, the bright orange Cr(VI) is reduced to Cr(III), which has a green coloration. In these oxidation reaction, the oxidizing agent is often just shown as [O].

Oxidation of Primary Alcohols:

Primary alcohols are oxidized in two steps, first forming aldehyde, and then carboxylic acid:

Ethanol (primary alcohol) + [O], heat 🡪 Ethanal (aldehyde) + [O], heat 🡪 Ethanoic acid (carboxylic acid)

The aldehyde can be removed via distillation since the aldehyde has a lower boiling point than the alcohol and the carboxylic acid (aldehydes cannot form hydrogen bonds between their molecules).

If the desired product is carboxylic acid, the aldehyde must be left in contact with the oxidizing agent for a long period of time in a reflux condenser.

Oxidation of Secondary Alcohols:

Secondary Alcohols are oxidized through heat and an oxidizing agent to ketones.

Example:

 Propan-2-ol + [O], heat, reflux condenser 🡪 Propanone

Oxidation of Tertiary Alcohols:

Tertiary alcohols are not oxidized under comparable conditions because oxidation would involve breaking the carbon skeleton since the tertiary carbon is connected to only the functional group and three alkyl groups. Breaking the carbon skeleton would require significantly more energy. The would be no orange-green color change in the reaction vessel.

10.5: Halogenoalkanes

10.5.1: Describe, using equations, the substitution reactions of halogenoalkanes with sodium hydroxide.

General formula: $C\_{n}H\_{2n+1}X$

In all halogenoalkanes, the halide group can be replaced by other atoms.

Halogenoalkanes lead to the production of CFC’s.

The carbon-halogen bond is polar due to charge distribution:
 For example: In the C-Cl bond, the carbon has a partial positive and the chlorine has a parial negative charge. The carbon is called the **electron deficient.** The electron deficient makes halogenoalkanes susceptible to imposition by **nucleophiles**, or species which are electron rich and therefore attracted to regions of electron deficiency.

Because halogenoalkanes are saturated molecules, they undergo substitution. In reactions with sodium hydroxide, the electron rich hydroxide ion will be attracted to the electron deficient carbon and thus substitute the halogen to which the carbon is bonded. This makes the halogenoalkane an alcohol.

These are called Sn reactions and their exact mechanisms differ depending on whether it is a primary, secondary, or tertiary halogenoalkane.

Primary Halogenoalkane: SN2 mechanism:

The first step is the **slow** one (rate-determining step), where the hydroxide ion is attracted to the electron deficient carbon. This leads to the unstable transition state in which the **halogen and the hydroxide ion are both partially bonded** to the carbon.

The transition state then quickly breaks down, releasing the halogen and forming the alcohol.

The reaction is considered bimolecular because the slow step in the reaction depends on the concentration of both the halogenoalkane and the hydroxide ion.

Tertiary Halogenoalkanes: SN1 mechanism:

The presence of three alkyl groups surrounding the electron deficient carbon causes **steric hindrance**, meaning that it is difficult for the hydroxide ion to attack the carbon.

 The first step of this reaction involves the halogenoalkane ionizing by breaking its carbon-halogen bond. This step happens in such a way such that the halogen acquires both electrons, leaving the carbon with a positive charge (this process is called heterolytic fission: $X:X\rightarrow X:^{-}+X^{+}$) (the process by which the carbon is left with a positive charge after ionization is called carbocation).

 The molecule in the intermediate cabocation stage is kept stable despite the ionized carbon’s positive charge by the three electron donating alkyl groups.

Since the slow step of the reaction mechanism is determined by the concentration of only the halogenoalkane, it is called unimolecular.

Note that both the SN2 and SN1 mechanisms involve heterolytic fission since the halogen is released as a negative ion.

Secondary halogenoalkanes undergo a mixture of both reaction mechanisms.

The reactivity of the halogenoalkanes depends on the strength of their respective C-Halogen bond. Therefore iodoalkane would most readily react while the fluoroalkane would not readily react.

10.6: Reaction Pathways:

Primary Alcohols 🡪 Aldehyde 🡪 Carboxylic Acids

Secondary Alcohols 🡪 Ketones

Alkene 🡪 Halogenoalkane 🡪 Dihalogenoalkane

Alkene 🡪 Halogenoalkane 🡪 Trihalogenoalkane/ Tetrahalogenoalkane

Alkene 🡪 Alkane

Halogenoalkane 🡪 Alcohol

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