

Introduction to organic functional groups and hydrocarbons biology essay



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Hydrocarbons are compounds made up entirely of carbon and hydrogen. The major types of hydrocarbons are alkanes, alkenes, alkynes, and aromatic compounds. Alkanes are parent compounds of all organic compounds and only composed of single bonds (C-H and C-C bonds). The linear (non cyclic) alkanes have a molecular formula of C_nH_{2n+2} . Alkanes that are cyclic (ring structure) are called cycloalkanes. For every ring that is present, there are two less hydrogen atoms than the equivalent (in terms of number carbons) linear alkane. Alkanes are non-polar and are the least reactive and simplest of all hydrocarbons. This is because alkanes do not have a functional group, which is usually the part of a compound that is reactive. There are very types of reactions that alkanes undergo such as reaction with oxygen and mostly all types of highly combustible substances. Alkanes are important as they are used in heating gases, gasoline, fuel oil, motor oil, jet fuel, paraffin, and many other types of fuels. 1

Alkenes are hydrocarbons with functional groups of at least one carbon-carbon double bond. The double bonds are the reactive part of an alkene. Double bonds are stiffer than single bonds and do not allow for rotation and thus create cis-trans (geometric) isomers. Alkenes have a molecular formula of C_nH_{2n} and relatively non-polar. Alkenes that are cyclic are called cycloalkenes. The formula that takes into account double bonds and number of rings is $C_nH_{2n+2-2(\text{number of rings} + \text{number of double bonds})}$. Alkenes are much more reactive than alkanes due to unsaturation (containing double bond) and can undergo combustion, halogen addition, hydrogenation, epoxidation, oxidative cleavage, and other non-specific free radical reactions. Alkenes are used for synthesis of polymers, drugs, pesticides, and

other valuable chemicals including ethanol, acetic acid, ethylene glycol, and vinyl chloride. The polymers are important in making a variety of products ranging from plastic bags to car bumpers. 1

Alkynes are hydrocarbons with functional groups of at least one carbon-carbon triple bond. Since the triple bond is linear, there is not geometric isomerism. This is the reason that cyclic alkynes (cycloalkynes) are very rare, and could only be present with eight or more carbons. Alkynes have a molecular formula of C_nH_{2n-2} . They are relatively non-polar and virtually insoluble in water. Alkynes have similar reactivity to alkenes and are able to undergo halogenations, hydrogenations, and oxidation. Acetylene is a very important type of alkyne as it is used as fuel for oxyacetylene welding torch and used as industrial feedstock. 1

Aromatic hydrocarbons are derivatives of benzene, a singular carbon ring with three double bonds. These compounds look like cycloalkenes but have differing properties. They are very stable due to large resonance energy. It is hard to hydrogenate these compounds to cyclohexane and can be only under forcing conditions. Oxidation also requires specific conditions.

Halogenations are possible, but only with the aid of catalysts. Though, they can undergo reaction with chloroform through a series of Friedel-Craft alkylations in the presence of anhydrous aluminum chloride. Charles Friedel and James Crafts discovered these reactions in 1877 and include alkylation reactions and acylation reactions. 2 Alkyl halides alkylate benzene to form alkylbenzenes in presence of Lewis acid catalysts. The alkylation is a part of electrophilic aromatic substitution reaction where an electrophile substitutes

for a hydrogen atom in an aromatic hydrocarbon to make a carbon-carbon
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double bond. The acylation part is similar to the alkylation except that the reagent is not an alkyl chloride and is instead an acyl chloride. 1

In this experiment, alkanes, alkenes, and aromatic compounds were put through various different tests to observe the outcome and help identify the class of an unknown substance. The tests include, physical appearance, odour, solubility in water and cyclohexane, test with bromine, test with aqueous potassium permanganate, and aluminum chloride with chloroform test. The different types of classes result in different products and can be distinguished from one another. The results of the tests on the unknown compound can be matched with the recorded observations of each class to help determine the hydrocarbon functional group of the unknown.

Experimental:

The experimental procedure carried out for this lab followed the steps listed in the lab manual. Refer to Organic Chemistry Lab Manual Fall 2010-Winter 2011 pages 34-39.

It was noted that among alkene and alkyne, an alkene compound was used as these two types of hydrocarbons exhibit very similar properties in terms of reactivity.

Results:

Table 1: Shows the compounds used to represent each class of hydrocarbons (alkanes, alkenes, and aromatic compounds) including an unknown compound and blanks. All the compounds were analyzed for their chemical and physical properties and underwent various types of tests and the

observations were recorded in the table below. To determine if a reaction occurred, the results of tests on each class were compared to that of the blanks, with a deviation in result leading to show that a reaction occurred.

Class:

Alkane

Alkene

Aromatic

Unknown

Blank

Compound Name:

n-Heptane

1-Octene

Naphthalene

#663

(Solvent Only)

Molecular Structure:

—

—

Chemical Formula:

C₇H₁₆

C₈H₁₆

C₁₀H₈

Physical Appearance

Liquid, transparent

Liquid, transparent

Solid, white, shiny

Liquid, transparent

—

Odour

No odour

Smells a bit strong

No odour

Slight odour

—

Solubility in Water

Insoluble

Insoluble

Insoluble

Insoluble

—

Solubility in Cyclohexane

Soluble

Soluble

Soluble

Soluble

—

Test with Br₂ in CH₂Cl₂

Light orange colour, transparent, no reaction

Clear solution (transparent), reaction occurred

Dark orange colour, no reaction

Dark orange colour, no reaction

The solution remained brown/orange

(control)

Illuminate Br₂ solution

White colour, translucent, reaction occurred (slow)

(Not necessary as a reaction was observed with Br₂ in CH₂Cl₂)

Light orange colour, no reaction

Translucent, clear, very light yellow, slight reaction

The solution remained brown/orange

(control)

Litmus Paper Test

pH= acidic (paper turned pink)

pH= neutral (no change in paper)

pH= acidic (paper turned pink)

pH= acidic (paper turned pink)

Paper stayed the same colour pH= neutral (control)

Test with aqueous KMnO_4 (Baeyer Test)

The solution remained purple (just darkened), no reaction

The solution turned brown, reaction occurred

The solution remained purple, no reaction

The solution remained purple, no reaction

The solution remained purple (control)

Test with AlCl_3 and Chloroform

The solution remained white and cloudy, no reaction

The solution remained white, no reaction

The solution turned blue, reaction occurred

The solution turned yellow, reaction occurred

The solution was white, and cloudy

(control)

Discussion:

The substances that were used to represent alkane, alkene, and aromatic compounds were n-heptane, 1-octene, and naphthalene, respectively. There

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was an unknown sample given which was tested alongside the different classes of hydrocarbons in order to deduce the functional group present based on the chemical and physical properties observed. The first test was the test of physical appearance. The alkane, alkene, and unknown products were all clear, transparent, and in liquid form, while the aromatic compound was white in colour, had a shiny texture, and was in a solid state. Colourless and white compounds are thought to be pure organic compounds and since the unknown was a colourless liquid, it was believed to be an organic compound. 3 The next test was that of odour. This task was difficult and is not believe to be a reliable test as the presence of a definite smell fluctuated in opinion between different experimenters. Only alkene seemed to have a very distinct and strong smell to it. It was hard to figure out the approximate type of smell of alkene as the compound was whiffed for a brief time due to precautionary safety measurements. Other compounds did not have a strong scent to them.

There were two solubility tests that were performed. Firstly, the compounds were tested for solubility in water. All the organic compounds were in soluble in water as water is a polar compound and the organic compounds are non-polar in nature. When water was added to the compounds, there were two distinct layers that formed every time, indicating insolubility. The compounds were then tested for solubility in cyclohexane (cyclic alkane), a non-polar compound. When a few drops of cyclohexane were added, all the organic samples seemed to dissolve readily and no layers were observed. The results observed were expected as all organic compounds are non-polar and would only be able to dissolve in non-polar substances. Since the unknown sample

behaved like the alkane, alkene, and aromatic compound in terms of polarity, it was to be concluded that the compound was indeed an organic compound (non-polar).

As a safety measurement, all the tests that followed were performed under the fumehood. Also, the whole experiment was performed wearing safety goggles, lab coat, and gloves as many chemicals are corrosive and toxic. The tests performed next also included a control (blank) in order to check for a reaction occurring by comparing the results of the organic compounds to that of the blanks.

When the organic compounds were tested with bromine in the presence of CH_2Cl_2 , only alkene sample reacted at first. It was observed that a reaction took place because the control remained a brownish orange colour, while the alkene sample turned clear. This made sense as alkenes readily undergo halogenation reaction (Refer to Figure 1). The bromine addition is usually a stereospecific anti-addition across the double bond of an alkene (1-octene in this case) that could be seen in Figure 2. ¹ This gave an indication that the unknown was not an alkene. The samples that did not initially react (even after warming) were subjected to illumination with the use of a sun lamp. It was noted that the alkane solution had a reaction occurring as it turned clear compared to the control which was still brownish orange in colour. This was probably due to the radical formation of bromine, from the energy provided by the light, that reacted with the C-H bonds. ¹ Refer to Figure 3 for a general reaction mechanism. Along with the control, aromatic and unknown compounds did not show a change in colour and remained brownish orange.

This could have been due to the fact that bromination is very selective and <https://assignbuster.com/introduction-to-organic-functional-groups-and-hydrocarbons-biology-essay/>

doesn't readily react with aromatic compounds. When the solutions were subjected to a litmus paper test, only alkene and the control showed no change in colour of the paper, concluding that they were of a neutral pH. Meanwhile, alkane, aromatic and unknown compounds all turned pink, showing that they all had an acidic pH. This indicated that there was a reaction due to the illumination of the Br₂ affected solutions. This was due to the formation of HBr (a strong acid) after the free radical bromination of alkanes and halogenations of aromatic compounds. Referring to Figure 4, there are three major and one minor product formed from the bromination of alkane (n-heptane) as secondary hydrogens are more reactive than primary ones. While in the aromatic, naphthalene compound, the bromine tends to attach to the tertiary carbon (refer to Figure 5). The halogenation of aromatic compound has substitution occurring between a tertiary hydrogen and bromine in order to retain all the original double bonds of the compound. After this test it was concluded that the unknown was more similar to alkane or aromatic compound and definitely not alkene.

Figure 1: A sample mechanism showing the addition of halogens to alkenes. First, there is an electrophilic attack by a halogen molecule that results into the formation of a halonium ion and a halide ion. The halonium ion is a three-membered ring with a positive charge on the halogen. The halide ion acts as a nucleophile and attacks the halonium ion from the back to open it up and attach itself to the carbon. This creates an overall anti-addition of halogens to the double bonds.

Figure 2: Reaction of 1-Octene (alkene) with Br₂ in the presence of CH₂Cl₂ results into two products.

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Figure 3: A general sample reaction mechanism of free radical halogenation. The mechanism is broken down into a series of steps that include initiation and propagation. During initiation, halogen (bromine) radicals are formed. Light provides sufficient energy to split a bromine molecule to form two bromine radicals. Propagation is divided into two steps. During the first step, one of the bromine radical reacts with alkane and abstracts hydrogen to form an alkyl radical and HBr (strong acid). In the second step, the alkyl radical reacts with a new molecule of bromine and abstracts a bromine to form a alkyl halogen and bromine radical.

Figure 4: Reaction of n-heptane with Br₂ results into four different products due to radical bromination. The first product (top most) shown is a minor product because the bromine takes place of a primary hydrogen. The rest of the products are major products because they all replace a secondary hydrogen. The more substituted the intermediate radical, the more stable the product.

Figure 5: Halogenation of Naphthalene with a bromine molecule in dichloromethane. This is a substitution reaction which retains all double bonds of the aromatic compound.

The organic compounds were all then tested with aqueous potassium permanganate (Baeyer test). The only sample that reacted was the one with the alkene as the solution turned brown when 95% ethanol and 2% potassium permanganate (in a drop-wise manner) were added. The alkene was oxidized and a diol was formed due to a syn addition of two hydroxyl groups across the double bond (refer to Figure 7). 1 This lead to the

formation of MnO_2 which in turn lead to the brown colour of the solution. 3 The alkane, aromatic, unknown, and control all remained purple as there was no reaction. Further oxidation would lead to an oxidative cleavage of the glycol (two hydroxyl groups) to form ketones and aldehydes, which forms acid. This test further proved that the unknown did not have a functional group of an alkene. This whole test is called the Baeyer test as the potassium permanganate is a Baeyer's reagent, discovered by Adolf von Baeyer, in order to test for presence of unsaturation (such as double bonds) in a compound. Refer to Figure 6 for a general reaction mechanism.

Figure 6: A general sample mechanism of permanganate hydroxylation of an alkene. The hydroxylation occurs with syn stereochemistry. Further oxidation of the product splits a carbon-carbon bond.

Figure 7: Reaction of 1-Octene with 2% potassium permanganate in 95% ethanol. Initially, the reaction results into a diol but further oxidation splits the product and leads to formation of an aldehyde.

The final test was of aluminum chloride with chloroform test. The aromatic and the unknown compounds were seen to have undergone a reaction as they had a change in colour (blue and light yellow, respectively) while the alkane, alkene, and control solutions remained white and cloudy. Since most of the tests determined that the unknown was not an alkene, this test proves that the unknown is not alkane, either and hence, it is aromatic. Aromatic compounds are known to go through Friedel-Craft alkylation in the presence of a proper catalyst (refer to Figure 8). As observed during the experiment, these types of reactions often yield in vibrant colours due to the

delocalization of charge among the aromatic rings of the compound. 3 In this experiment, the addition of chloroform to naphthalene with aluminum chloride as a catalyst caused a reaction (refer to Figure 9).

Figure 8: A sample general mechanism of Friedel-Crafts Alkylation, an electrophilic aromatic substitution. During the first step, a carbocation is formed. In the second step, an electrophilic attack from a benzene forms a sigma complex (resonating structure). In the last step, a proton is lost from the sigma complex to reform the aromatic ring to result into an alkylated product of benzene.

Figure 9: A reaction of Naphthalene with chloroform in the presence of aluminum chloride in a series of Friedel-Craft Alkylations.

Thus, based on the experiment performed and the comparisons made, the unknown sample #663 was found to contain a functional group of an aromatic compound. There were probably some sources of errors while performing the experiment. One of the sources of errors was that the measurements were all taken as an approximate as there were no indicators on the pipettes while transferring liquids and the solid compounds were not weighed. Furthermore, the pipettes that were used to transfer the liquids from the main containers could have been contaminated as they were shared. The impurities were probably the reason for some of the solutions having a very slight change in colour despite not reacting.

Questions:

R

S

Figure 104: Shows the structure of (-)-trans-carveol with chiral centers that are circled and labeled as having S or R configuration.

Refer to Figure 10. The chiral centers are circled and they are classified as S or R configuration shown by the arrows point to them.

Figure 11: Hydrogenation reaction of trans-carveol. The reaction formula translates to $C_{10}H_{16}O + 2H_2 \rightarrow C_{10}H_{20}O$.

Moles of $C_{10}H_{16}O$: = mass of $C_{10}H_{16}O$ / molar mass of $C_{10}H_{16}O$

$$= 27.2g / 152g/mol$$

$$= 0.179mol$$

Moles of H_2 : ratio of $C_{10}H_{16}O / H_2$ = moles of $C_{10}H_{16}O / H_2$

$$1 / 2 = 0.179mol / mol H_2$$

$$H_2 = 0.358mol$$

Volume of H_2 : $PV = nRT$

$$(1atm)(V) = (0.358mol)(0.08206 L atm K^{-1} mol^{-1})(273.15 K)$$

$$V = 8.02 L$$

Therefore, 8.02×10^3 mL volume of H_2 needed for hydrogenate 27.2g of trans-carveol at STP.

Figure 12: Extensive hydroboration reaction of trans-carveol results into two products.

Litmus paper is made up of an indicator called Litmus, which is a water-soluble mixture of 10-15 dyes that are extracted from Lichens and many other types of natural plants such as red cabbage and absorbed onto a filter paper. Litmus paper is used as an acid-base indicator based on pH values. The dyes respond differently to different pH by changing colour. Paper indicates alkaline (basic) solutions by turning blue and indicates acidic solutions by turning red. There are slight variations in colour that relate to different ranges of pH values but blue and red colours are sufficient to determine if a solution is acidic or basic. This test was discovered around 1300 AD by Amaldus de Villa Nova, a Spanish alchemist. A regular use of litmus paper is to test and regulate the pH level in swimming pools and spa.

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