EXPERIMENT 0

Organic Compounds: Alkanes

A. Goal

The goal of this laboratory experiment is to practice unit conversions and carry out calculations with the correct number of significant figures.

B. Materials

 \square This is theory-based experiment.

C. Background

Alkanes

This first section will introduce organic chemistry, covering the most simple organic compounds: the alkanes. Alkanes—also called hydrocarbons—are simply made of carbon and hydrogen with all C-C bonds being single bonds. First, you will be introduced to a few organic chemicals and you will learn about a series of different organic formulas that can represent the same compound. Then, you will learn the basic naming rule of alkanes, which extend to other—more complex—organic chemicals.

Molecular formula for alkanes

The naming of alkanes results from the combination of a prefix and a suffix. On one hand, the suffix is always *ane*. On the other hand, the prefix depends on the number of carbons in the molecule. Table ?? shows a list of the different prefixes. For example, the alkane with a single carbon is called methane (CH_4). Other examples of alkanes are ethane that contains two carbons (C_2H_6) or propane with three carbons (C_3H_8). The molecular formula for an alkane with n carbon atoms is:

$$C_n H_{2n+2} \tag{1}$$

Hence, we have that the molecular formula for methane (n = 1) is CH_4 and the molecular formula for octane (n = 8) is C_8H_{18} . Molecular formulas represent only the molecular compositions, showing only the elements in the molecule.

A review of the different structural formulas

At this point, you have seen four different ways to represent organic molecules. Using propane as example, here all the formulas: We have that the *molecular formula* (e.g. C₃H₈ for propane) is mainly used to indicate the composition of the molecule in the form of Carbon and Hydrogen atoms. A second way to represent propane is using its *expanded structural formula*, that is by representing all atoms in the molecule and all atomic connections. A third molecular representation is the *condensed structural formula* that uses CH₃ and CH₂ units, only representing the C-C bonds. Finally, the *skeletal formula* is perhaps the most simplistic representation as only the C-C bonds are represented in the form of simple lines. It is important to understand that *all formulas are just different ways to represent the same molecule*.

Sample Problem 1

Write down the condensed and skeletal formulas for heptane.

SOLUTION

Heptane has seven carbons, hence its condensed formula will have two CH3 units and five CH2 units:

$$H_3C$$
C H_2 C H_2 C H_2 C H_3

The skeletal formula for would be:



STUDY CHECK

Draw the skeletal formula of decane.

Table 1 Prefixed for alkane naming			
# Carbons	prefix	# Carbons	prefix
1	Meth	6	Hex
2	Eth	7	Hepta
3	Prop	8	Octa
4	But	9	Nona
5	Pent	10	Deca

Cycloalkanes

Alkanes are perfect examples of hydrocarbons, with C-C chains and all carbon atoms saturated with hydrogen. Cycloalkanes are simply alkanes with a cyclic structure. We will cover the molecular, condensed, and skeletal formulas for these chemicals.

Cyclic alkanes

Consider the expanded structure of hexane. A cycloalkane results from removing the left and right hydrogen while connecting the molecule in the form of a cycle:

$$\begin{array}{c} H \\ H - C - CH_2 - CH_2 - CH_2 - CH_2 - CH_2 - CH_2 \\ \end{array}$$

As the most stable structure for six lines is the hexagon, the resulting structure of cyclohexanes would be:

Naming cycloalkanes

The naming of alkanes and cycloalkanes is very similar. You just need to add the cyclo prefix to the name. For example, the alkane with five carbons is called pentane, whereas the corresponding cycloalkane is called cyclopentane:

$$\begin{array}{cccc} \operatorname{CH_2}^{-\operatorname{CH_2}} & & & \\ & & \operatorname{CH_2}^{-\operatorname{CH_2}} & & \operatorname{Cyclopentane} \end{array}$$

Alkanes with substituents

Oftentimes alkanes have other groups of atoms called substituents attached to the hydrocarbon chain. This section covers the naming of alkanes with substituents. Here is an example of an alkane and an alkane with a substituent:

$$\begin{array}{ccc} H & NO_2 \\ | & | \\ CH_2-CH_2-CH_3 & CH_2-CH_2-CH_3 \\ \hline Propane & Nitropropane \end{array}$$

In the substituted molecule, a nitro group has replaced a hydrogen atom.

Substituents

There are many different substituents—also called groups—that can be found attached to an alkane chain. Their names are indicated in Table 1. The easiest substituents are halogens; atoms of chorine (Cl—), bromine (Br—) or iodine (I—) can replace hydrogen atoms in an alkane. The name of these substituents—chloro, bromo and iodo—resembles the name of the corresponding atom. Other substituents can contain carbon, like a methyl (CH_3 —) or a ethyl (CH_3 CH₂—). There are even more complex substituents such as tert-butyl in which a central carbon atom is connected to three different methyl groups. The name of substituents (methyl) comes from the name of the alkane (methane) by replacing the *-ane* suffix with *-yl*.

Naming rules for branched alkanes

Overall, the rules to name branched alkanes are:

- 1 Step one: Look for the longest carbon-carbon chain that will give the ending name of the molecule (e.g. four carbons would be butane).
- 2 **Step two:** Number the main chain starting at the end closest to the substituents so that the numbers for the substituents are small.
- 3 **Step three:** Name the substituents with their position and order them alphabetically.

Sample Problem 2

Name the following hydrocarbon:

$$\begin{array}{c} CH_{3} \\ I \\ CH_{3} - CH_{2} - C - CH_{3} \\ I \\ CH_{2} - CH_{2} - CH_{3} \end{array}$$

SOLUTION

First we locate the longest chain. We have five possible chains, and the longest one has six carbons. Hence the name of the hydrocarbon would be hexane. Now we need to number the carbons so that we start numbering the closes to the substituents the possible.

$$\begin{array}{c} \operatorname{CH_3} \\ \operatorname{CH_3-CH_2-C-CH_3} \\ 1 & 2 & \stackrel{|3}{\underset{CH_2-CH_2-CH_3}{\cup}} \\ & & 4 & 5 & 6 \end{array}$$

We have two methyl connected to carbon number three. Hence the final name will be:

Answer: 3-dimethylhexane.

STUDY CHECK

Name the following hydrocarbon:

$$\begin{array}{c} \operatorname{CH}_2-\operatorname{CH}_2-\operatorname{CH}_2-\operatorname{CH}_3\\ \operatorname{CH}_3-\operatorname{CH}_2-\operatorname{C}-\operatorname{CH}_3\\ \operatorname{CH}_2-\operatorname{CH}_2-\operatorname{CH}_3 \end{array}$$

Molecular diversity

You have certainly taken painkillers for a headache or over-the-counter drugs to get over a cold. Maybe you drink coffee and perhaps you like tea. All these substances contain active organic molecules. These active molecules are hydrocarbon derivatives and differ from plain hydrocarbons, which are simply made of carbon and hydrogen. Active molecules contain functional groups such as alcohol, ethers, carboxylic acids, amines, amides, or aromatic groups. These groups of atoms have a specific function and give activity to the molecule. The goal of this section is simply to identify the different groups.

Table 2 Names of so	everal functional group	os			
Functional group	Name	Functional group	Name	Functional group	Name
$\begin{array}{c} \hline R_1 \\ R_2 \\ \end{array} \begin{array}{c} R_3 \\ R_4 \end{array}$	Alkene	O R-C-R'	Ketone	R-ОН	Alcohol
$R-C\equiv C-R'$	Alkyne	R-C-H	Aldehyde	R-SH	Thiol
O R-C-OH	Carboxylic acid	R' R-N-R"	Amine	R-O-R'	Ether
$^{\mathrm{O}}_{\mathrm{R-C-O-R'}}$	Ester	$\begin{matrix} \mathrm{O} & \mathrm{R''} \\ \mathrm{II} & \mathrm{I} \\ \mathrm{R} - \mathrm{C} - \mathrm{N} - \mathrm{R'} \end{matrix}$	Amide		Phenyl

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Pre-lab Questions

Organic Compounds: Alkanes

CH_4	_		C ₂ H ₆	
C_4H_{10}	_		C ₃ H ₈	
C_5H_{12}	_		C ₉ H ₂₀	
ven the foll	owing molecu	lar formula, name the follow	ving cyclic alkanes (hydrocarbons)):
C_3H_6	_		C_6H_{12}	
C_4H_8	_		C_7H_{14}	
C_5H_{10}	_		C ₉ H ₁₈	
dicate the m	nolecular, expa	anded, condensed and skeleta	al formula for the following linear	alkanes:
	Molecular	Expanded Formula	Condensed Formula	Skeletal Formula
	Formula			
Hexane				
Pentane				
entify the fu	unctional group	ps:		
-	unctional grou	-		
entify the fu	ınctional grou	ps: Functional Group	Molecule	Functional Group
-	unctional grou	-		
-	0	-		
-	0 0	-	Molecule H ₃ C CH ₂ CH C CH ₂	
-	O II C	-		
Molecule	0 0	-		
-	0 0	-		
Molecule	0 0	-		

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Results EXPERIMENT

Organic Compounds: Alkanes

Linear Alkanes Use the molecular models set for this experiment. Each sphere represents an element. Carbon is black, hydrogen white, oxygen red and nitrogen blue. Build up the following molecules and complete the table. Show your professor all molecular models before proceeding to next part.

	Expanded Formula	Condensed Formula	Skeletal Formula
Methane			N/A
Ethane			
Propane			
Butane			

Cyclic Alkanes Use the molecular models set for this experiment. Each sphere represents an element. Carbon is
black, hydrogen white, oxygen red and nitrogen blue. Build up the following molecules and complete the table. Show
your professor all molecular models before proceeding to next part.

	Expanded Formula	Condensed Formula	Skeletal Formula
Cyclopropane			
Cyclobutane			
Cyclopentane			
Cyclohexane			

Short alkanes with substituents Use the molecular models set for this experiment. Each sphere represents an element. Carbon is black, hydrogen white, oxygen red and nitrogen blue. Build up the following molecules and complete the table. Show your professor all molecular models before proceeding to next part.

	Expanded Formula	Molecular Formula
Chloromethane		
Dichloromethane		
BromoChloro -Fluoromethane		
Chloroethane		

Long alkanes with substituents Use the molecular models set for this experiment. Each sphere represents an element. Carbon is black, hydrogen white, oxygen red and nitrogen blue. Build up the following molecules and complete the table. Show your professor all molecular models before proceeding to next part.

Name	Condensed Formula	Skeletal Formula
	$\begin{array}{c} \operatorname{CH}_3 \\ \operatorname{CH}_3 - \operatorname{CH} - \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname{CH}_3 \end{array}$	
	$\begin{array}{ccc} \operatorname{CH}_3 & \operatorname{CH}_3 \\ & \mid & \mid \\ \operatorname{CH}_3 - \operatorname{CH} - \operatorname{CH} - \operatorname{CH}_2 - \operatorname{CH}_3 \end{array}$	

More alkanes with substituents There is no need to use the molecular models at this point. Now, name the following molecules:

Formula	name
$\begin{array}{ccc} \operatorname{Br} & \operatorname{Cl} \\ \operatorname{CH}_3 - \operatorname{CH} - \operatorname{CH} - \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname{CH}_3 \end{array}$	
$\begin{array}{c} \operatorname{CH_2-CH_3} \\ \vdash \\ \operatorname{CH_3-CH-CH_2-CH_2-CH_3} \end{array}$	
$\begin{array}{c} {\rm CH_3} \\ {\rm CH_3 - C - CH_2 - CH_2 - CH_3} \\ {\rm CH_2 - CH_3} \end{array}$	

Functional Groups Identity the following functional groups:

Formula	name
H_3C O I C	
$\overset{\mathrm{NH}_{2}}{\bigcirc}$	
ОН	
$\begin{array}{ccc} H & CH_2 & CH_3 \\ C & CH_2 & \end{array}$	
ОН	