

Nomenclature of Simple Organic Compounds: A Study Assignment

Performance Goal

27-1 Within the limits discussed in this exercise, give the name derived from the provided organic structure, or draw the structure from the name.

INTRODUCTION

This study assignment presents a brief introduction to International Union of Pure and Applied Chemistry (IUPAC) nomenclature rules and some common names. The rules selected here are by no means a comprehensive treatment of IUPAC nomenclature, and several areas have been neglected for the sake of simplicity. The areas not covered include: multifunctional organic compounds, complex substituents, stereochemistry, aromatic heterocyclic common names, and complex functional groups. Omitting polyfunctional organic nomenclature also eliminates the need to assign priorities to functional groups. The lab is designed with allied health students in mind and is not directed at chemistry majors.

The student must be familiar with stick diagrams to complete the lab.

CHEMICAL OVERVIEW

The IUPAC committee devised a way to systematically name organic molecules. This lab will outline how to name monofunctional organic molecules. Because of their frequency of use, some common names have also been added.

The process of assigning a name to an organic molecule has been broken down into a series of rules as outlined below.

ALKANES

Straight chain alkanes are named with a prefix that refers to the number of carbons and then adding the -ane suffix (see Table 27.1).

Branched alkanes and all other organic molecules are named according to a series of rules.

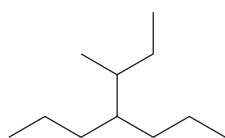
Table 27.1 Nomenclature of straight chain alkanes

Carbon Chain Length	Prefix	Alkane Name
1	meth-	methane
2	eth-	ethane
3	prop-	propane
4	but-	butane
5	pent-	pentane
6	hex-	hexane
7	hept-	heptane
8	oct-	octane
9	non-	nonane
10	dec-	decane

Rule 1. Find the longest contiguous chain in the molecule and name it.

- A.** If there are two chains of identical length, choose the one that contains the largest number of substituents.

Example 1



base is heptane
3-methyl-4-propylheptane



base is hexane
2,4,4-trimethylhexane

- B.** If a principal functional group is present, select the longest chain that includes that functional group.

Rule 2. Name all groups attached to the longest chain as substituents.

- A.** Alkyl substituents are named by dropping the -ane from the name and adding the suffix -yl. For example, methane becomes methyl, and ethane becomes ethyl (see Figure 27.1).
- B.** If there are identical substituents, number them and add the prefix di, tri, tetra, etc., to indicate the number of times that they appear.
- C.** Halogens are named as substituents such as fluoro-, chloro-, bromo-, and iodo-.

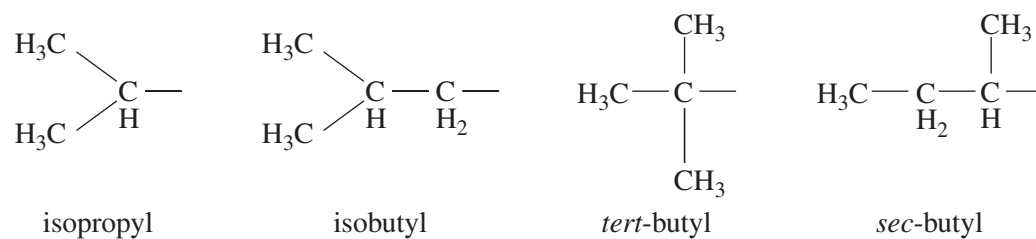
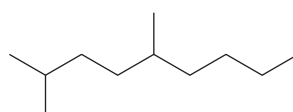
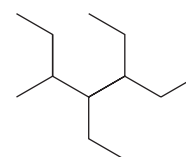


Figure 27.1
Common names of alkyl substituents

Example 2



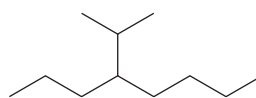
2,5-dimethylnonane



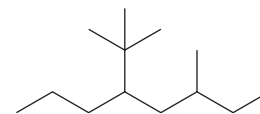
3,4-diethyl-5-methylheptane

D. Some substituents are given common names as outlined in the table below.

Example 3



4-isopropyloctane

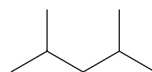


5-tert-butyl-3-methyloctane

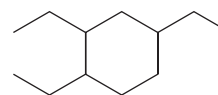
Rule 3. Number the carbons of the longest chain, beginning with the end that is closest to a substituent.

- In the case of two substituents being numbered the same, number according to alphabetical order.
- If a principal functional group is present, assign the smallest number possible to that functional group.
- A comma is used to separate numbers of identical substituents.

Example 4



2,4-dimethylpentane

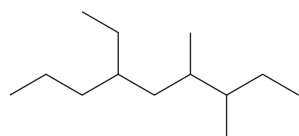


1,2,4-triethylcyclohexane

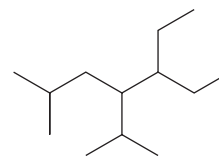
Rule 4. Write the name of the principal chain. Then arrange all of the substituents in alphabetical order (each preceded by the carbon number to which it is attached and a hyphen) and then add the name of the stem. The prefixes referring to the number of substituents such as di-, tri-, tetra-, are

ignored in alphabetizing. The prefix iso- is not ignored but tert- and sec- are.

Example 5



6-ethyl-3,4-dimethylnonane



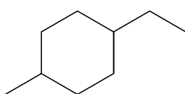
5-ethyl-4-isopropyl-2-methylheptane

CYCLIC STRUCTURES

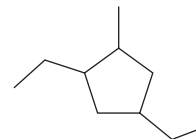
Rule 5. Cyclic structures are designated by the prefix cyclo-.

- A.** Numbering cyclic structures depends on the number of substituents on the ring. If the structure contains two substituents, they are numbered alphabetically. Three or more substituents are numbered by assigning the order that gives the lowest possible number to all of the substituents.

Example 6



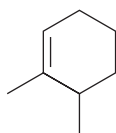
1-ethyl-4-methylcyclohexane



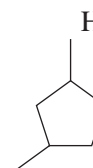
1,4-diethyl-2-methylcyclopentane

- B.** If a principal functional group is present, it gets priority and is numbered first.

Example 7



1,6-dimethylcyclohex-1-ene



3-methylcyclopentanol

AROMATIC COMPOUNDS

Rule 6. Aromatic rings are named and numbered in the same fashion as cyclic structures.

A. However, common names are often used to denote benzene derivatives as shown in Figure 27.2.

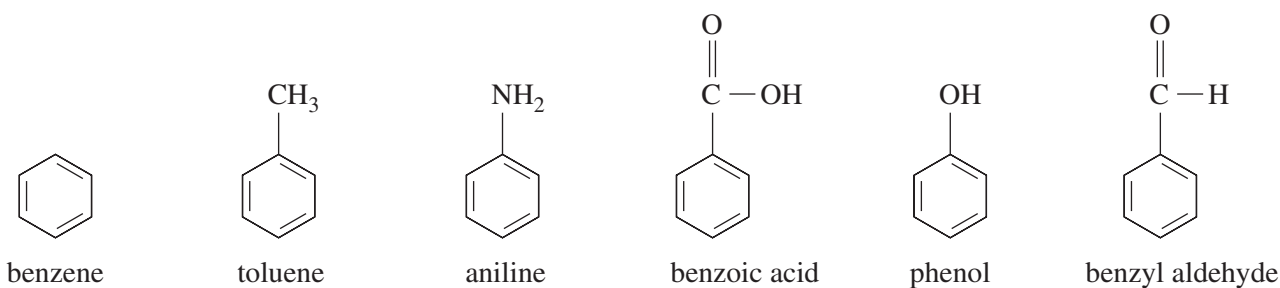
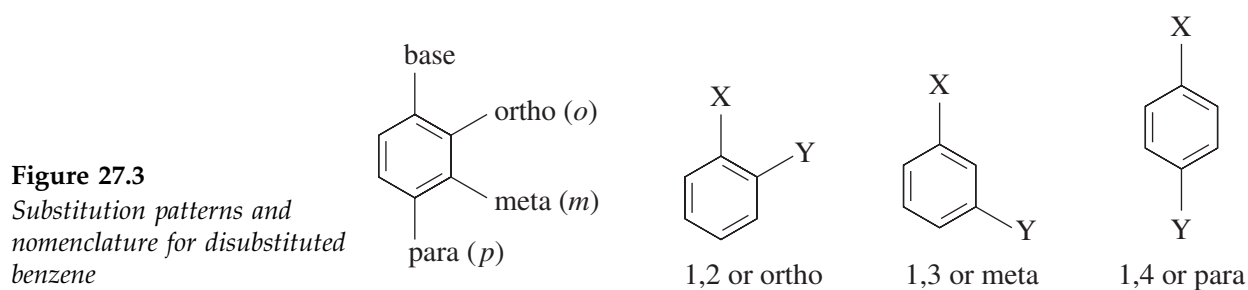


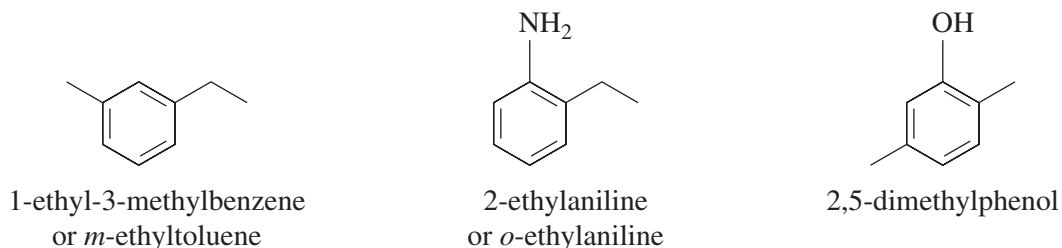
Figure 27.2

Common names of benzene derivatives

B. In addition, there is a method to denote the substitution pattern of disubstituted benzene rings by using the prefixes ortho-, meta-, and para-, which are abbreviated *o*-, *m*-, and *p*-. The substitution patterns are outlined in Figure 27.3.



Example 8



FUNCTIONAL GROUPS

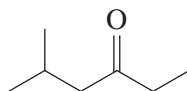
Rule 7. Suffixes identify the principal functional group or class to which the molecule belongs (see Table 27.1). Some functional groups such as amines, amides, ethers, and esters also utilize prefixes to denote the entire

Table 27.2 Nomenclature rules for functional groups

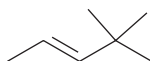
Functional Group	Suffix and Prefix	Functional Group	Suffix and Prefix
1. Alkane $\begin{array}{c} \text{R} & & \text{R} \\ & \diagdown & / \\ & \text{C}-\text{C} & \\ & / & \diagdown \\ \text{R} & & \text{R} \end{array}$	-ane	8. Ketone $\begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{R} \end{array}$	-one
2. Alkene $\begin{array}{c} \text{R} & & \text{R} \\ & \diagdown & / \\ & \text{C}=\text{C} & \\ & / & \diagdown \\ \text{R} & & \text{R} \end{array}$	-ene	9. Carboxylic acid $\begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{OH} \end{array}$	-oic acid
3. Alkyne $\text{R}-\text{C}\equiv\text{C}-\text{R}$	-yne	10. Ester $\begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{OR}' \end{array}$	name R', main chain -oate
4. Halide $\text{R}-\text{X}$ $\text{X} = \text{F}, \text{Cl}, \text{Br}, \text{I}$	-o	11. Amine $\begin{array}{c} \text{R}' \\ \\ \text{R}-\text{N} \\ \\ \text{R}' \end{array}$	N-R' group, main chain, amine
5. Alcohol $\text{R}-\text{OH}$	-ol	12. Amide $\begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{N} \\ \quad \\ \text{R}' \quad \text{R}' \end{array}$	N-R' group, main chain, -amide
6. Aldehyde $\begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{H} \end{array}$	-al	13. Thiol $\text{R}-\text{S}-\text{H}$	main chain -thiol
7. Ether $\text{R}-\text{O}-\text{R}$	shorter chain -oxy, main chain		

functional group. All of the suffixes and prefixes for a select list of principal functional groups are listed in Table 27.2.

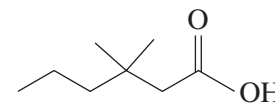
- A. When numbering and naming a compound, the principal functional group takes precedence. Thus, the principal functional group is always included in the base chain and is numbered so that the principal functional group is assigned the lowest number possible.
- B. Some functional groups are numbered in front of the suffix instead of the root word. This occurs when the functional group can appear at variable positions. Terminal functional groups, such as aldehydes, carboxylic acids, esters, and amides, are numbered 1 as long as they are the principal functional group. The number 1 is usually omitted for these groups.
- C. When adding a suffix to the root, if two vowels appear together, the first vowel is dropped.

Example 9

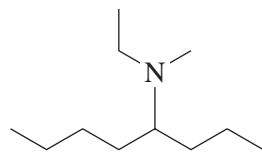
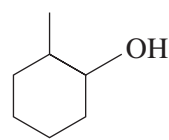
5-methylhexan-3-one



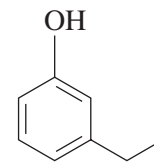
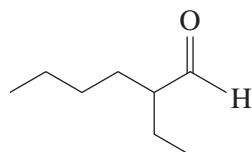
4,4-dimethylpent-2-ene

3,3-dimethylhexanoic acid
(carboxylic acid is terminal
always number 1)

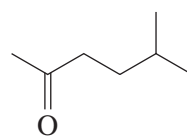
Example 10

*N*-ethyl-*N*-methyloctan-4-amine

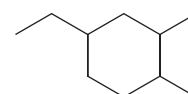
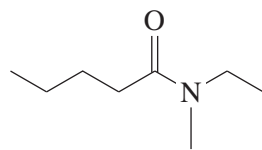
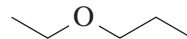
2-methylcyclohexanol

3-ethylphenol
m-ethylphenol

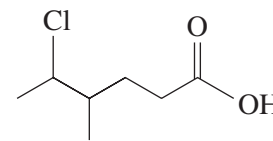
2-ethylhexanal



5-methylhexan-2-one

4-ethyl-1,
2-dimethylcyclohexane*N*-ethyl-*N*-methylpentanamide

1-ethoxypropane



5-chloro-4-methylhexanoic acid

Name _____

Date _____

Section _____

Experiment 27

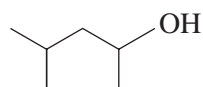
Advance Study Assignment

1. Write the names that correspond to the following structures.

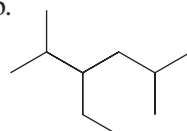
Structure

Name

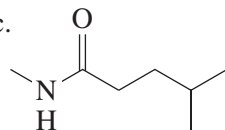
a.



b.



c.



2. Write the structures that correspond to the following names.

Name

Structure

a. 2-ethoxybutane

b. 3-methylcyclohexanone

c. 4-methylhexanal

Name _____

Date _____

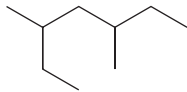
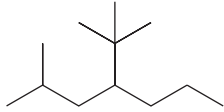
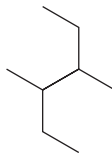
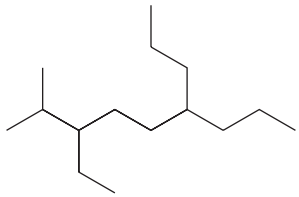
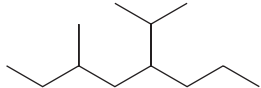
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Experiment 27

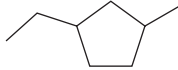
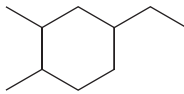
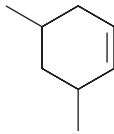
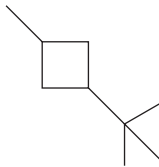
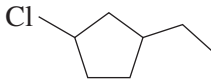
Work Page

General Instructions: For each substance whose name is given, write the structure; if the structure is given, write the name.

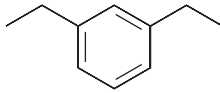
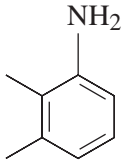
Alkanes

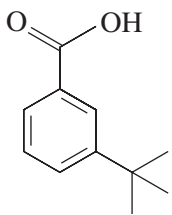
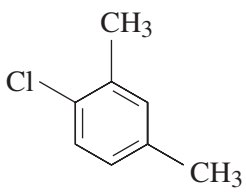
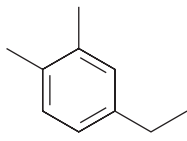
	2,2-dimethylpentane
	6-ethyl-4-isopropyl-3-methyloctane
	3-ethyl-3,4-dimethylhexane
	2,3,5-trimethylhexane
	4- <i>tert</i> -butyl-3,5-diethylheptane

Cyclic Structures

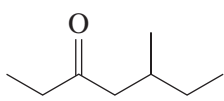
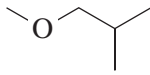
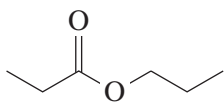
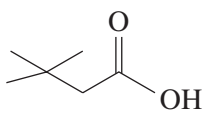
	1,1-dimethylcycloheptane
	1,2,3-trimethylcyclopropane
	1-ethyl-3-isopropylcyclopentane
	4-fluorocyclohex-1-ene
	1-ethyl-3-methylcyclobutane

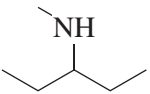
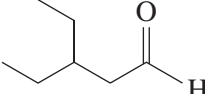
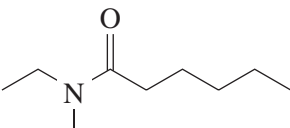
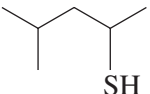
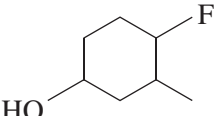
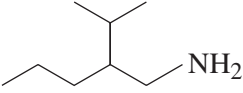
Aromatic Compounds

	<i>o</i> -ethyltoluene
	3-chlorophenol

	1-ethyl-3,5-dimethylbenzene
	<i>p</i> -isopropylbenzaldehyde
	5-ethyl-2,3-dimethylphenol

Functional Groups

	4-methylpent-2-yne
	methyl 2-methylbutanoate
	2-propylcyclopentanone
	<i>N</i> -ethyl- <i>N</i> -methylethanamine

	N-methylpentanamide
	3-fluoro-4-methylpentanoic acid
	3,4-dimethylpentanal
	1-methoxypropane
	2,4-dimethylpentan-3-ol
	2-chloro-3,4,5,5-tetramethylhex-2-ene

Name _____

Date _____

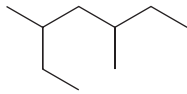
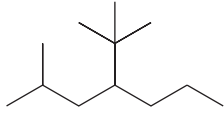
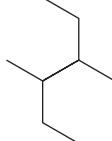
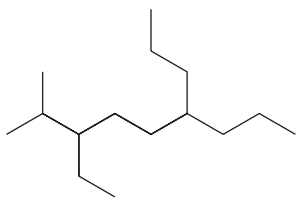
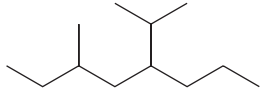
Section _____

Experiment 27

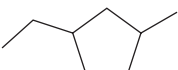
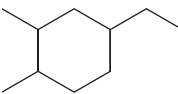
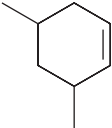
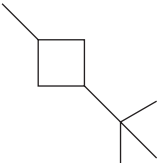
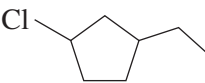
Report Sheet

General Instructions: For each substance whose name is given, write the structure; if the structure is given, write the name.

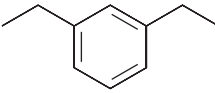
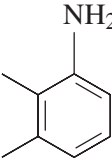
Alkanes

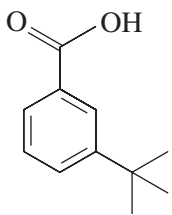
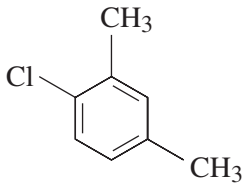
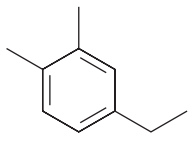
	2,2-dimethylpentane
	6-ethyl-4-isopropyl-3-methyloctane
	3-ethyl-3,4-dimethylhexane
	2,3,5-trimethylhexane
	4- <i>tert</i> -butyl-3,5-diethylheptane

Cyclic Structures

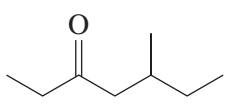
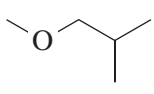
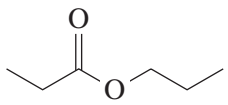
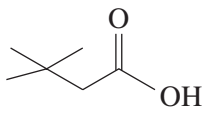
	1,1-dimethylcycloheptane
	1,2,3-trimethylcyclopropane
	1-ethyl-3-isopropylcyclopentane
	4-fluorocyclohex-1-ene
	1-ethyl-3-methylcyclobutane

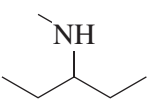
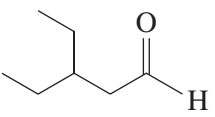
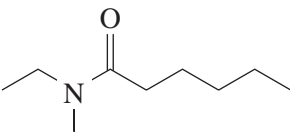
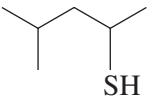
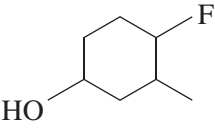
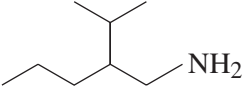
Aromatic Compounds

	<i>o</i> -ethyltoluene
	3-chlorophenol

	1-ethyl-3,5-dimethylbenzene
	<i>p</i> -isopropylbenzaldehyde
	5-ethyl-2,3-dimethylphenol

Functional Groups

	4-methylpent-2-yne
	methyl 2-methylbutanoate
	2-propylcyclopentanone
	<i>N</i> -ethyl- <i>N</i> -methylethanamine

	N-methylpentanamide
	3-fluoro-4-methylpentanoic acid
	3,4-dimethylpentanal
	1-methoxypropane
	2,4-dimethylpentan-3-ol
	2-chloro-3,4,5,5-tetramethylhex-2-ene