Organic Chemistry

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CONTENTS

OVERVIEW

- Chemists coined the term **organic** to distinguish between compounds obtained from living organisms and those obtained from mineral sources
- Carbon is the central atom in the study of organic chemistry [1] because the carbon atom can form four bonds. They can bond to form chains, rings, spheres, sheets, and tubes of almost any size and can form combinations of single, double, and triple covalent bonds.
- **Terminal carbon** is where the chain of carbon ends

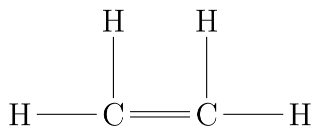
FUNCTIONAL GROUPS

- Compounds fall into **organic families** [2]
- The physical properties and reactivity of the compounds are related to these combinations, called **functional groups** [3]
- Thus, if we can identify the functional group a organic compound belongs to, we can predict the properties of the molecule

Each functional group can be composed of **3 different types of components**

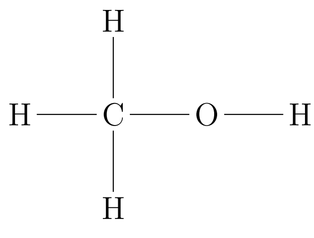
1. Carbon-carbon multiple bonds (single, double, and triple bonds). The diagram below shows the double bond between two carbons in ethene

ethene, C_2H_4



2. Single bonds between a carbon atom and a more electronegative atom. For instance, a C−O, a C−N bond, or a C−Cl bond. The diagram below shows the bond between carbon and oxygen

methanol (an alcohol), CH_3OH



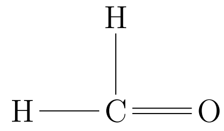
3. Carbon atom bonded to an oxygen atom, −C=O. The diagram below shows the double bond between carbon and oxygen

[1] **Organic chemistry:** the study of compounds in which carbon is the principle element.

[2] **Organic family:** a group of organic compounds with common structural features that impart characteristic physical properties and reactivity

[3] **Functional groups:** these groups determine whether the molecules are readily soluble in polar or non-polar solvents, whether they have high or low melting/boiling points, and whether they readily react with other molecules

methanal (an aldehyde), CHOH



Carbon-Carbon Multiple Bonds

- C-C single bonds are not as reactive as double and triple bonds
- The second and third bonds (the π-bonds) are more reactive than the first bond (the σ-bond). This allows carbon-carbon multiple bonds to be sites for reactions in which more atoms are added to the C atoms

Single Bonds Between Carbon and More Electronegative Atoms

- When a C atom is bonded to a more electronegative atom, the molecule is polar (most of the time)
- Polar molecules are stronger, which is why CH_4 is gas at room temperature while CH_3OH is liquid at room temperature
- If the O or N atoms are in turn bonded to an H atom, an $-$OH or $-$NH group is formed. The prescence of an $-$OH group enables an organic molecule to form hydrogen bonds with other $-$OH groups, increasing intermolecular attraction and enabling these molecules to mix readily with polar solutes and solvents

Double Bonded Carbon and Oxygen

- The double covalent bond between C and O requires that four electrons be shared between the atoms, all four being more strongly attracted to the O atom
- This makes the C=O bond strongly polarized, increasing the effects of high melting and boiling points and increasing solubility in polar solvents
- What is the effect of the prescence of an $-$OH group or an $-$NH group on
  (a) The melting and boiling points of the molecule?
  (b) The solubility of the molecule in polar solvents?
- Identify all components of functional groups in the following structural diagrams. Predict the solubility of each substance in water
  (a) $CH_3{-}O{-}H$
  (b) $CH_3CH{=}CHCH_3$
  (c) $CH_3CH{=}O$
  (d) $CH_3CH_2COH{=}O$

Problems

1. Explain the meaning of the term "functional group"
2. Are double and triple bonds between C atoms more reactive or less reactive than single bonds?
3. Describe the three main components of functional groups in organic molecules

Solutions

1. A group/pattern of atoms that display consistent properties and reactivity regardless of the exact molecule they are found in. These functional groups help define the physical and chemical characteristics of an organic compound
2. Double and triple bonds between C atoms are more reactive than single bonds because the second and third bonds are π bonds which are much more reactive than the first bond which is a σ bond
3. The three main components are carbon carbon multiple bonds, single bonds between carbon and a more electronegative element, and carbon bonding with oxygen
4. (a) The melting and boiling points would increase because the molecule becomes more polar increasing the intermolecular force of attraction
   (b) The solubility in polar solvents would increase because the molecule is more polar
5. (a) There is a single bond between carbon and oxygen, making the molecule polar; this molecule is soluble in polar solvents
   (b) There is a double bond between two carbon atoms. This molecule is not soluble in water
   (c) There is a double bond between a carbon atom and an oxygen atom, making the molecule very polar; this molecule is very soluble in polar solvents
   (d) There is a single and double bond between carbon and two oxygens, making this molecule extremely polar; this molecule is extremely soluble in polar solvents

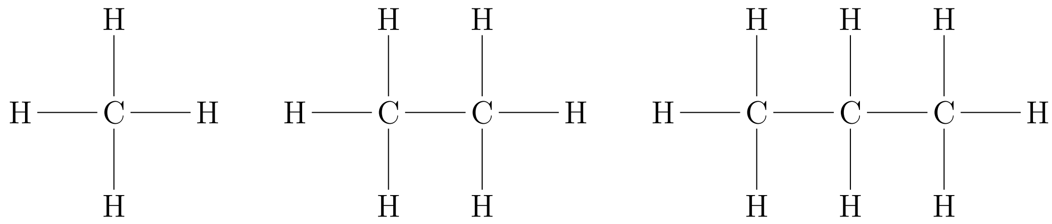
ALKANES AND THEIR ISOMERS

The simplest organic compounds are in the **alkane family**, and contain only carbon-carbon and carbon-hydrogen **single bonds**, but do not have any specific functional group. Hydrocarbons containing at least one carbon-carbon double bond are in the **alkene family**, while hydrocarbons containing at least one carbon-carbon triple bond are in the **alkyne family**.

Important. Alkanes are sometimes referred to as **saturated hydrocarbons**. Saturated [a] , in this case, means that each carbon atom is bonded to four other atoms (hydrogen or carbon)–the most possible; there are no double or triple bonds in these molecules. Saturated fats and oils are organic molecules that do not have carbon-to-carbon double/triple bonds.

[a] **Saturated:** (of an organic molecule) containing the greatest possible number of hydrogen atoms, and so having no carbon-carbon double or triple bonds, by definition.

Table 0.1: The three simplest alkanes. The pattern is that they each differ by a CH_2 unit, called **methylene**



Methane, CH_4 Ethane, C_2H_6 Propane, C_3H_8

[4]

Table 0.2: Alkanes and Related Alkyl Groups

Prefix	IUPAC Name	Formula	Alkyl Group	Alkyl Formula
meth-	methane	$CH_{4(g)}$	methyl-	$-CH_3$
eth-	ethane	$C_2H_{6(g)}$	ethyl-	$-C_2H_5$
prop-	propane	$C_3H_{8(g)}$	prop-	$-C_3H_7$
but-	butane	$C_4H_{10(g)}$	butyl-	$-C_4H_9$
pent-	pentane	$C_5H_{12(\ell)}$	pentyl-	$-C_5H_{11}$
hex-	hexane	$C_6H_{14(\ell)}$	hexyl-	$-C_6H_{13}$
hept-	heptane	$C_7H_{16(\ell)}$	heptyl-	$-C_7H_{15}$
oct-	octane	$C_8H_{18(\ell)}$	octyl-	$-C_8H_{17}$
non-	nonane	$C_9H_{20(\ell)}$	nonyl-	$-C_9H_{19}$
dec-	decane	$C_{10}H_{22(\ell)}$	decyl-	$-C_{10}H_{21}$

There are also common names when it comes to naming propyl groups and butyl groups. For the propyl group, there is *n*-propyl and isopropyl, shown below. The prefix *n*- (normal) refers to a straight-chain alkyl group, the point of attachment being at the terminal carbon. The isomer of the *n*-propyl group is the isopropyl group.

n-propyl (normal propyl) isopropyl

The common names for the butyl groups are shown below

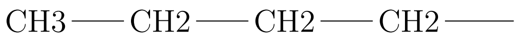
Isomers

Isomers are elements that have the **same molecular formula** but different structural formulas and properties.

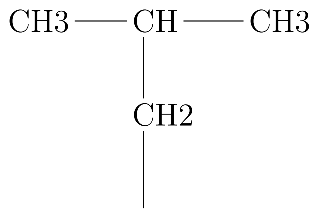
Alkanes that contain one continuous chain of linked carbons are called **straight-chain** alkanes. As the number of carbons in a chain increases beyond three, the arrangement of atoms

[4]**Methylene:** a single CH_2 unit in an organic compound.

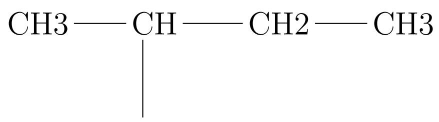
n-butyl



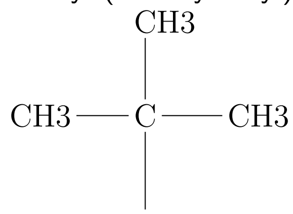
isobutyl



s-butyl (secondary butyl)

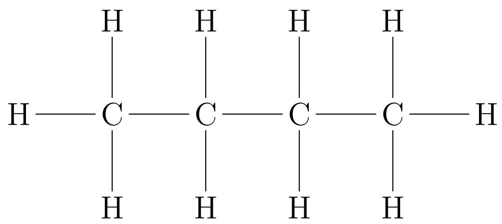


t-butyl (tertiary butyl)

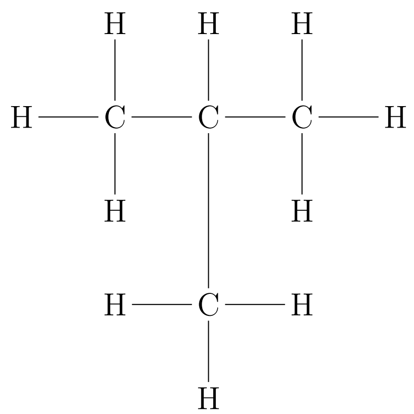


can expand to include **branched-chain** alkanes.

For instance, consider butane (C_4H_{10}), which is a straight-chain alkane



However, there is also 2-mehtylpropane (also called isobutane), which is a branched-chain alkane that has the same chemical formula as butane, but a different structural formula



Although these two molecules have the same chemical formula, they have different structural formulas and different chemical properties.
The four-carbon straight chain alkane butane may also be drawn with different bends or kinks in the backbone because the groups can freely rotate about the C-C bonds. This doesn't change the identity of the compound, but is rather a different representation of it
Pentane, which has molecular formula C_5H_{12}, has two branched-chain isomers, namely isopentane and neopentane. Pentane is a straight-chain alkane, while isopentane and neopentane are branch-chain alkanes. The prefix *neo* for neopentane is from the Greek work *neos*, meaning "new".

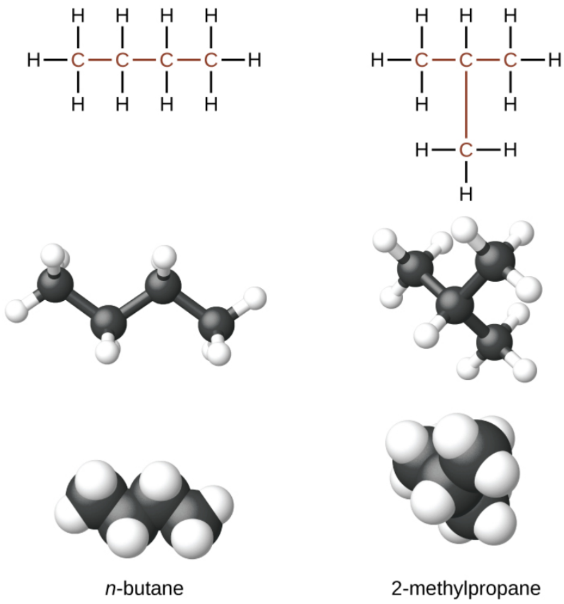


Figure 1: n-butane and 2-methylpropane are structural isomers. The butane is prefixed with a *n* as a short for the term *normal* to refer to a chain of carbon atoms without branching

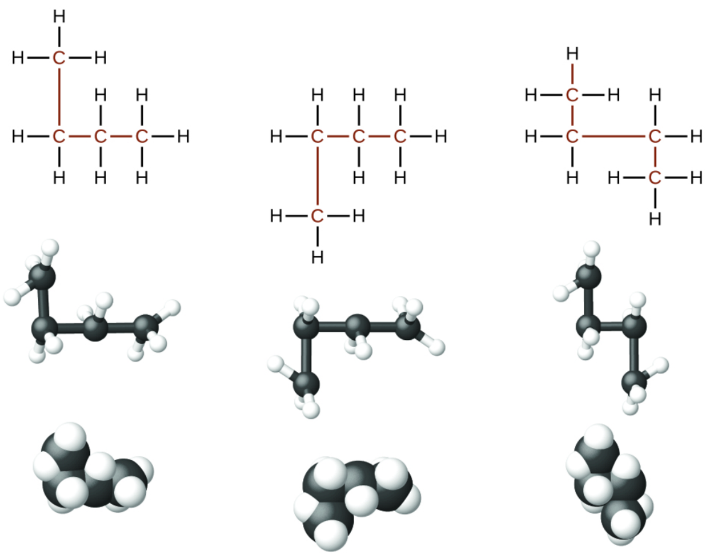
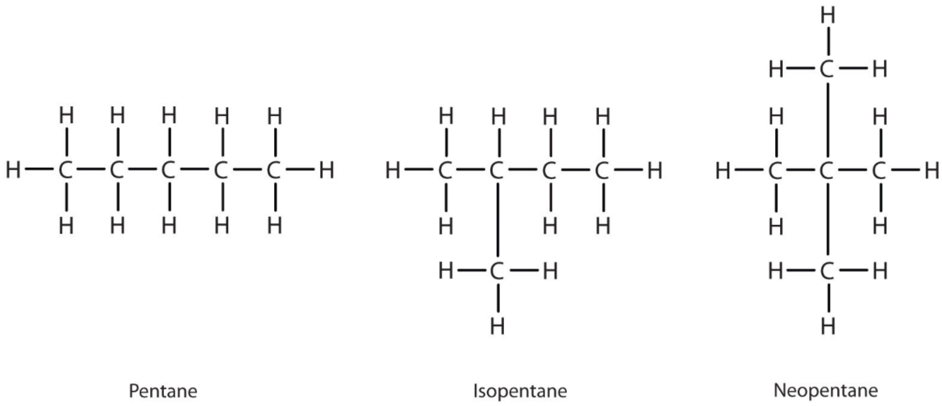


Figure 2: These three representations of n-butane are not isomers because they all contain the same arrangement of atoms and bonds

Important. A continuous (unbranched) chain of carbon atoms is called a straight-chain even though the tetrahedral arrangement about each carbon is a zigzag shape. Straight-chain alkanes are sometimes called *normal alkanes*.

Naming Alkanes

In the IUPAC system, a compound is named according to the number of carbons in the longest continuous chain (LCC) or parent chain and the family it belongs to. Atoms or groups



attached to this carbon chain, called *substituents* [5] , are then named, with their positions indicated by a numerical prefix at the beginning of the name

Prefix (substituent) – Parent (# carbons) – Suffix (family name)

2-methyl prop ane → 2-methylpropane

Table 0.3: Parent name for 1-10 carbons and example alkanes

# of Carbons	LCC Name	Example Alkane	Condensed Structural Formula
1	*meth-*	methane	CH_4
2	*eth-*	ethane	CH_3CH_3
3	*prop-*	propane	$CH_3CH_2CH_3$
4	*but-*	butane	$CH_3CH_2CH_2CH_3$
5	*pent-*	pentane	$CH_3CH_2CH_2CH_2CH_2CH_3$
6	*hex-*	hexane	$CH_3CH_2CH_2CH_2CH_2CH_2CH_3$
7	*hept-*	heptane	$CH_3CH_2CH_2CH_2CH_2CH_2CH_3$
8	*oct-*	octane	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$
9	*non-*	nonane	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$
10	*dec-*	decane	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$

HYDROCARBONS

Hydrocarbons are organic compounds that contains only carbon and hydrogen atoms in its molecular structure. Hydrocarbons are classified by the kinds of carbon-carbon bonds in their molecules. In **alkanes** [6], all carbons are bonded to each other by single bonds, resulting in the maximum number of hydrogen atoms bonded to each carbon atom. These molecules are thus called **saturated hydrocarbons**. There are also **alkenes** [7] and **alkynes** [8] , which are organic molecules with double and triple bonds, respectively.

[5]**Substituent:** atoms or groups of atoms that branch off the parent chain.
[6]**Alkane:** a hydrocarbon with only single bonds between carbon atoms.
[7]**Alkene:** a hydrocarbon that contains at least one carbon-carbon double bond; general formula C_nH_{2n}
[8]**Alkyne:** a hydrocarbon that contains at least one carbon-carbon triple bond; general formula C_nH_{2n-2}

Important. In all of these hydrocarbons, the carbon-carbon backbone may form a straight chain, one or more branched chains, or a cyclic structure. All of these molecules are included in a group called **aliphatic hydrocarbons** [a]

[a]**Aliphatic hydrocarbon:** a hydrocarbon that has a structure based on straight or branched chains or rings of carbon atoms; does not include aromatic compounds such as benzene.

A hydrocarbon that is attached to the parent branch is called an **alkyl group** [9]. When *methane* is attached to the main chain of a molecule, it is called a *methyl* group, $-CH_3$. An *ethyl* group is CH_3CH_2, the branch formed when *ethane* links to another chain.

A fourth group of hydrocarbons with characteristic properties and structures is called the **aromatic hydrocarbons** [10]. The simplest aromatic hydrocarbon is benzene; all other members of this family are derivatives of benzene. The formula for benzene is C_6H_6, and the six carbons form a unique ring structure. Unlike cyclohexane, C_6H_{12}, the benzene ring has a planar structure, and is unsaturated. The bonds in the benzene ring have properties intermediate between single bonds and double bonds; the common structure shows a hexagon with an inscribed circle, symbolizing the prescence of double bonds in unspecified locations within the six-carbon ring. See Figure 3.

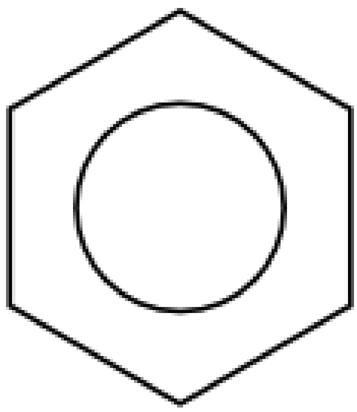


Figure 3: Benzene, C_6H_6, is a colourless, flammable, toxic, and carcinogenic, and has a pleasant odour. It is widely used in the manufacturing of plastics, dyes, synethetic rubber, and drugs.

CYCLIC HYDROCARBONS

In these compounds, the carbon atoms are connected in such a way to form a ring. It could be considered that the ends of the carbon chain connect; therefore, there are no terminal carbons. As a result, numbering the ring can start at carbon within the ring structure.

- To determine whether we use the straight-chain name or the cyclic chain, determine which one has more carbons
- Cycloalkanes are named by prefixing "cyclo-"

[9]**Alkyl group:** a hydrocarbon derived from an alkene by the removal of a hydrogen atom; often a substituent group or branch of an organic molecule.

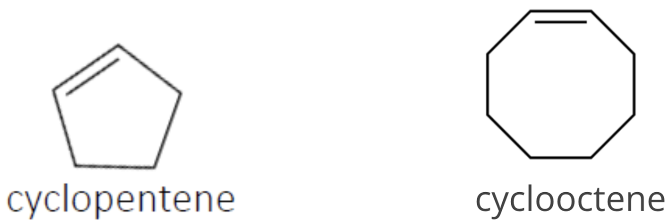
[10]**Aromatic hydrocarbons:** a compound with a structure based on benzene: a ring of six carbon atoms.

Table 0.4: Examples of hydrocarbons

Hydrocarbon group	Example	Formula
	Aliphatic	
alkane	ethane	CH_2CH_3
	cyclohexane	C_6H_{12}
alkene	ethene	CH_2CH_2
alkyne	ethyne	CHCH
	Aromatic	
	benzene	C_6H_6

Cycloalkenes

- When there is only 1 double bond in the ring and there are no substituent groups, it is not necessary to specify the location of the double bond



- For substituted cycloalkenes, number the ring in such a way that the carbon atoms of the double bond are in the 1- and 2- positions and that also gives the substituents the lower number at the first point of difference

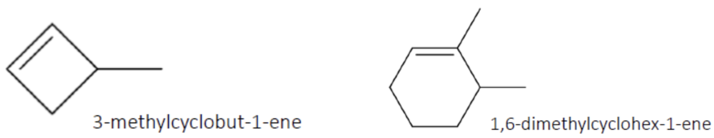


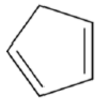
Figure 4: When there is a branch, the location of the double bond is also noted (always "-1")

- For cycloalkenes that contain more than one double bond, follow the rules used for alkenes
  - Number in the ring in such a way that the carbon atoms of the double bonds result in the lowest first point of difference. Location numbers must be provided
  - If the double bonds don't have a first point of difference, then use the substituent groups
  - If the groups result in the same substituent numbers, order by alphabetical order

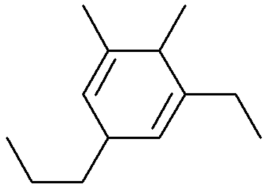
ALKENES AND ALKYNES

Alkenes

A subgroup of hydrocarbons that contain one or more carbon-carbon double bonds.



cyclopenta-1,3-diene



1-ethyl-5,6-dimethyl-3-propylcyclohexa-1,4-diene

1. For alkenes, the parent chain is identified by selecting the longest carbon chain that contains both C atoms of the carbon-carbon double bond
2. Then, select the appropriate prefix to indicate the total number of carbon atoms in the parent chain and use the suffix "-ene" to indicate the presence of a double bond

Alkynes

A subgroup of hydrocarbons that contain one or more carbon-carbon triple bonds.

1. For alkenes, the parent chain is identified by selecting the longest carbon chain that contains both C atoms of the carbon-carbon triple bond
2. Then, select the appropriate prefix to indicate the total number of carbon atoms in the parent chain and use the suffix "-yne" to indicate the presence of a triple bond

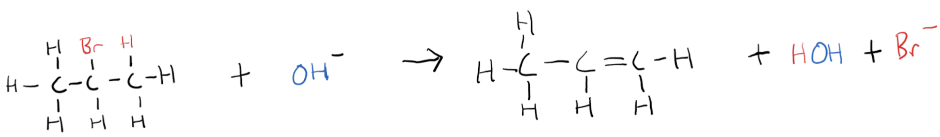
REACTIONS OF ALKANES, ALKENES, AND ALKYNES

Reaction of Alkanes

- Alkanes are less reactive than alkenes and alkynes
- Due to the saturated nature of alkanes, **substitution reactions** [11] are most common
- Halogen atoms can replace hydrogen atoms on the compound

Elimination Reactions to Produce Alkenes

In basic conditions (denoted by the OH^-), a halide ion and hydrogen atom are eliminated from adjacent carbons, also producing water



[11]**Substitution reactions:** Hydrogen atoms can be replaced by halogen atoms, one at a time, when an alkane reacts with F_2, Cl_2, or Br_2 in the prescence of UV light. Additional substitutions can occur if more halogen molecules are present.

Important. Generally, alkenes and alkynes are more reactive than alkanes. Alkenes and alkynes are unsaturated; therefore, they can accomodate additional atoms when the triple and/or double bonds break-these types of reactions are called **addition** reactions.