Organic Chemistry

Alkanes

by
Nurlin Abu Samah, Dr. Md. Shaheen & Dr. Nadeem Akhtar
Faculty of Industrial Sciences & Technology
nurlin@ump.edu.my

Chapter Description

- Aims
  - The students should **understand** the fundamental of organic chemistry in terms of alkanes
  - The students should be able to **explain** the fundamental of organic chemistry in terms of alkanes

- Expected Outcomes
  - Explain the basic knowledge in alkanes
  - Describe the chemical reactions and conditions for alkanes reactions
  - Describe the chemical reactions involving alkanes in certain industrial application

- References

  - Janice Gorzynski Smith (2008), Organic chemistry,Mc Graw-Hill
  - T. W. Graham Solomons. (2008). Organic chemistry, 9th ed, Mc Graw-Hill
  - K. Peter C. Vollhardt, Neil E. Schore, (2009). Organic chemistry, Fourth Edition: Structure and Function, Pub Chem

Alkanes

Introduction

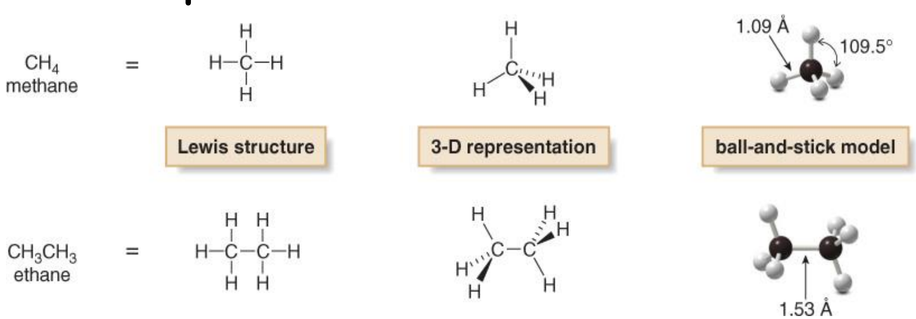
- Recall that alkanes are aliphatic hydrocarbons having C—C and C—H σ bonds. They can be categorized as acyclic or cyclic.
- Alicyclic alkanes have the molecular formula C_nH_{2n+2} (where n = an integer) and contain only linear and branched chains of carbon atoms. They are also called saturated hydrocarbons because they have the maximum number of hydrogen atoms per carbon.
- Cycloalkanes contain carbons joined in one or more rings. Their general formula is C_nH_{2n}, they have two fewer H atoms than an acyclic alkane with the same number of carbons.

Alkanes

Introduction

- All C atoms in an alkane are surrounded by four groups, making them sp^3 hybridized and tetrahedral shape, and all bond angles are 109.5°.

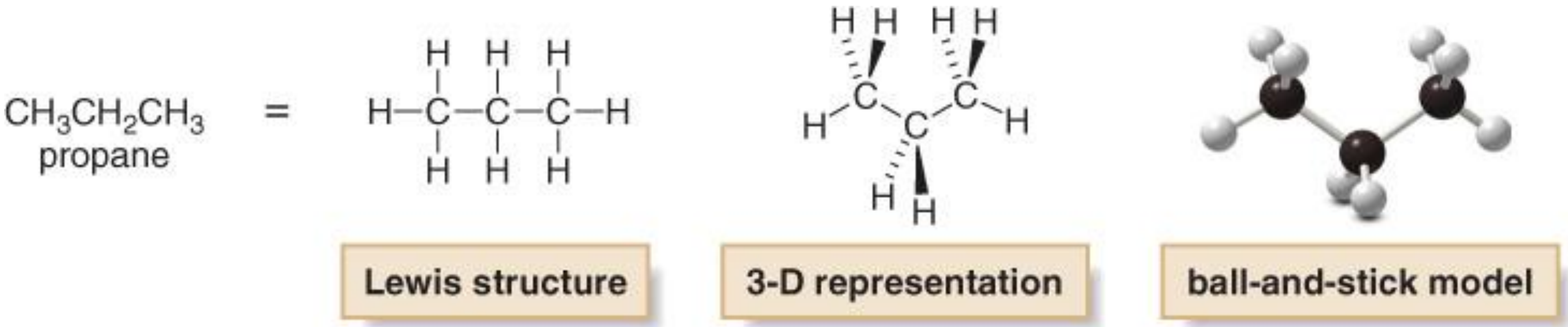
- The 3-D representations and ball-and-stick models for these alkanes indicate the tetrahedral geometry around each C atom. In contrast, the Lewis structures are not meant to imply any 3-D arrangement. Additionally, in propane and higher molecular weight alkanes, the carbon skeleton can be drawn in a variety of ways and still represent the same molecule.



Alkanes

Introduction

- The three-carbon alkane $CH_3CH_2CH_3$, called propane, has a molecular formula C_3H_8. Note in the 3-D drawing that each C atom has two bonds in the plane (solid lines), one bond in front (on a wedge) and one bond behind the plane (on a dashed line).



Alkanes

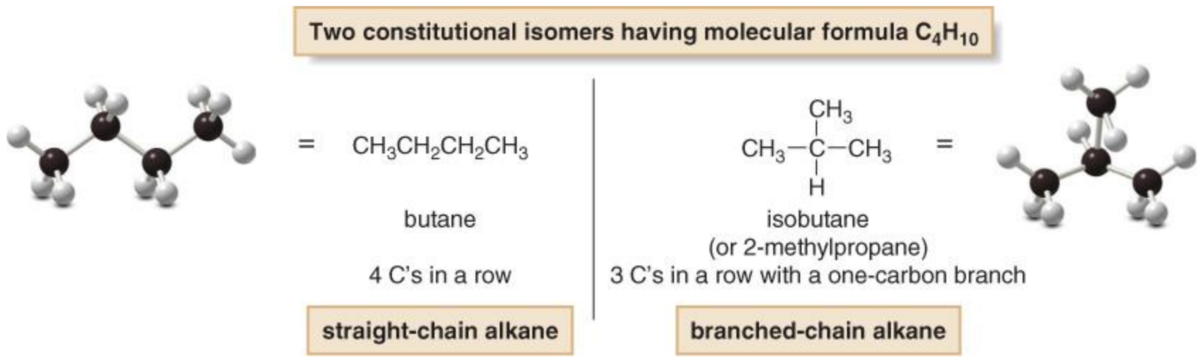
Introduction

- In propane and higher molecular weight alkanes, the carbon skeleton can be drawn in a variety of ways and still represent the same molecule. For example, the three carbons of propane can be drawn in a horizontal row or with a bend. These representations are equivalent.
- In a Lewis structure, the bends in a carbon chain don't matter.

Alkanes

Introduction

- There are two different ways to arrange four carbons, giving two compounds with molecular formula C_4H_{10}, named butane and isobutane.
- Butane and isobutane are isomers—two different compounds with the same molecular formula. Specifically, they are constitutional or structural isomers.
- Constitutional isomers differ in the way the atoms are connected to each other.

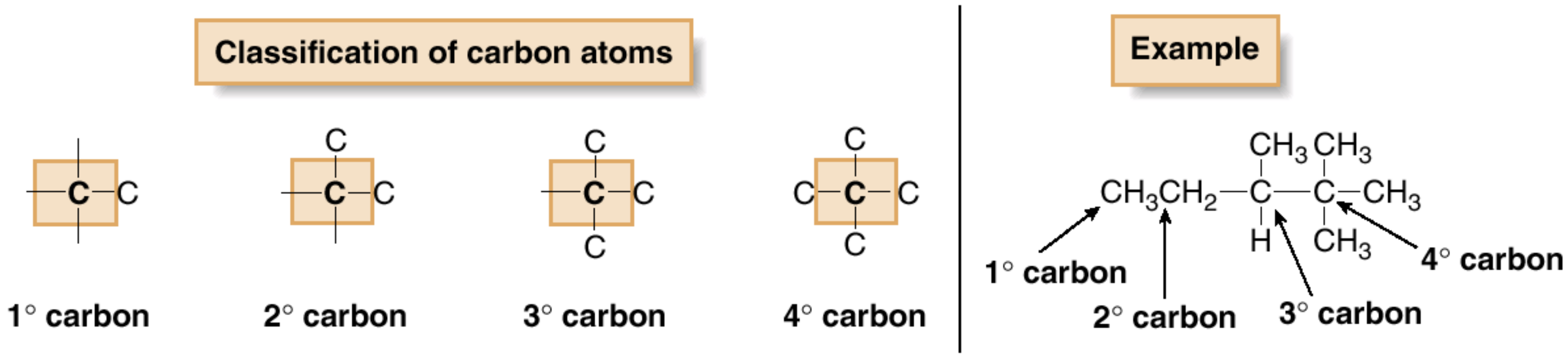


Alkanes

Introduction

- Carbon atoms in alkanes and other organic compounds are classified by the number of other carbons directly bonded to them.

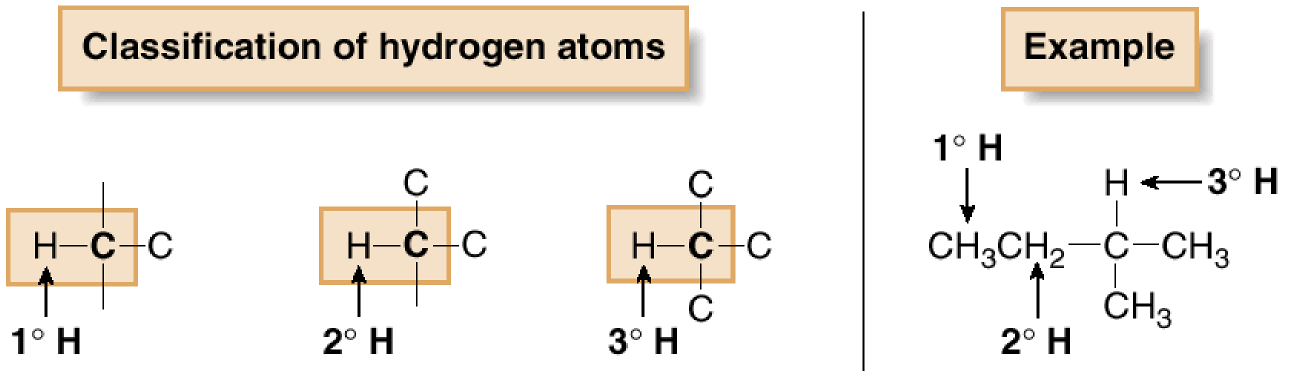
- A *primary carbon* (1° carbon) is bonded to *one* other C atom.
- A *secondary carbon* (2° carbon) is bonded to *two* other C atoms.
- A *tertiary carbon* (3° carbon) is bonded to *three* other C atoms.
- A *quaternary carbon* (4° carbon) is bonded to *four* other C atoms.



Introduction

- Hydrogen atoms are classified as primary (1°), secondary (2°), or tertiary (3°) depending on the type of carbon atom to which they are bonded.

- A *primary hydrogen* (1° H) is on a C bonded to one other C atom.
- A *secondary hydrogen* (2° H) is on a C bonded to two other C atoms.
- A *tertiary hydrogen* (3° H) is on a C bonded to three other C atoms.



Introduction

- The maximum number of possible constitutional isomers increases dramatically as the number of carbon atoms in the alkane increases.
- By increasing the number of carbons in an alkane by a CH_2 group, one obtains a "homologous series" of alkanes. The CH_2 group is called "methylene."

Alkanes

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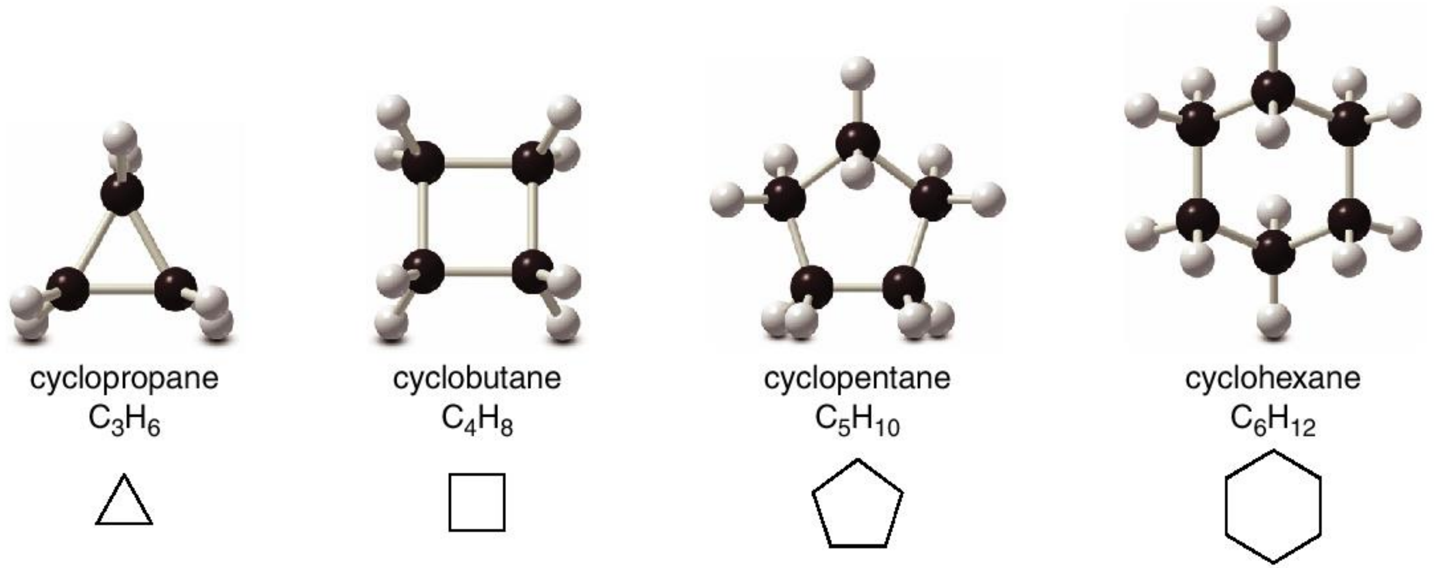
Number of C atoms	Molecular formula	Name (*n*-alkane)	Number of constitutional isomers
1	CH_4	methane	—
2	C_2H_6	ethane	—
3	C_3H_8	propane	—
4	C_4H_{10}	butane	2
5	C_5H_{12}	pentane	3
6	C_6H_{14}	hexane	5
7	C_7H_{16}	heptane	9
8	C_8H_{18}	octane	18
9	C_9H_{20}	nonane	35
10	$C_{10}H_{22}$	decane	75

Undecane (C11)
Dodecane (C12)
Tridecnae (C13)

Alkanes

Cycloalkanes

Cycloalkanes have molecular formula C_nH_{2n} and contain carbon atoms arranged in a ring. Simple cycloalkanes are named by adding the prefix *cyclo*- to the name of the acyclic alkane having the same number of carbons.



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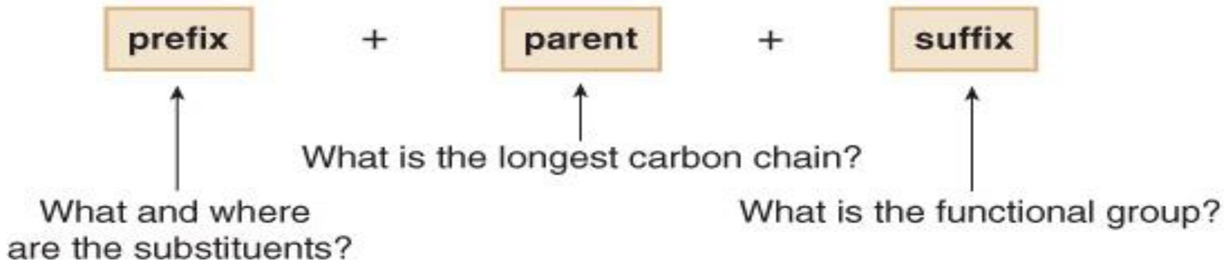
Nomenclature

The name of every organic molecule has 3 parts:

- The parent name indicates the number of carbons in the longest continuous chain.
- The suffix indicates what functional group is present.
- The prefix tells us the identity, location, and number of substituents attached to the carbon chain.

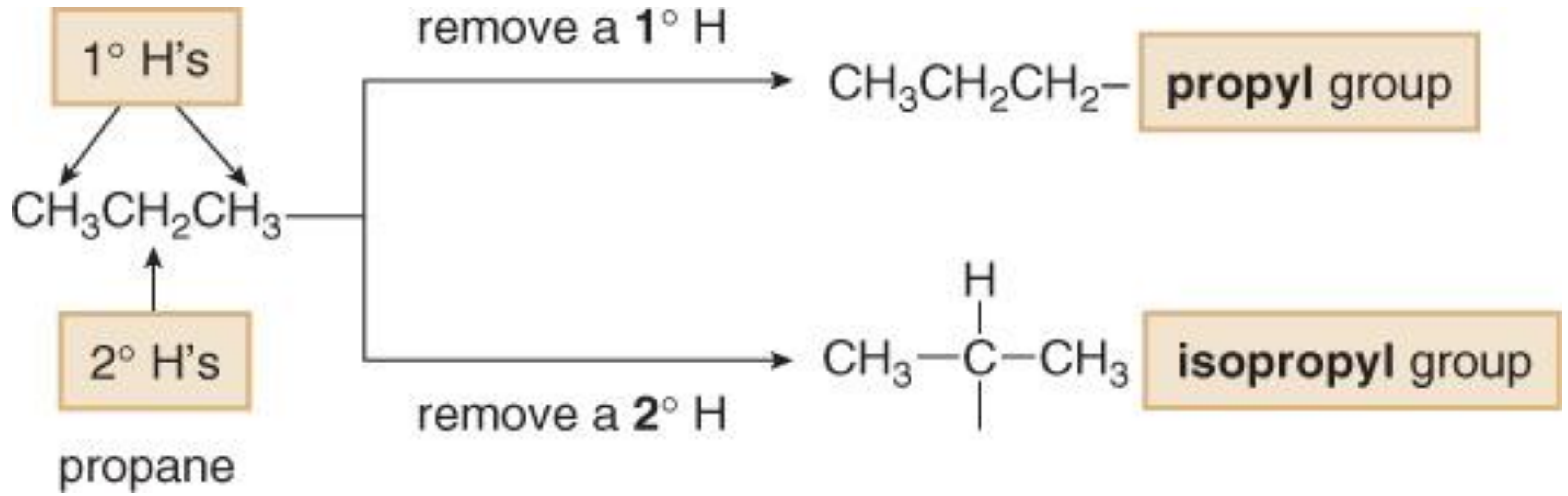


Nomenclature

- Carbon substituents bonded to a long carbon chain are called alkyl groups.
- An alkyl group is formed by removing one H atom from an alkane.
- To name an alkyl group, change the *–ane* ending of the parent alkane to *–yl*. Thus, methane (CH_4) becomes methyl (CH_3-) and ethane (CH_3CH_3) becomes ethyl (CH_3CH_2-).

Nomenclature

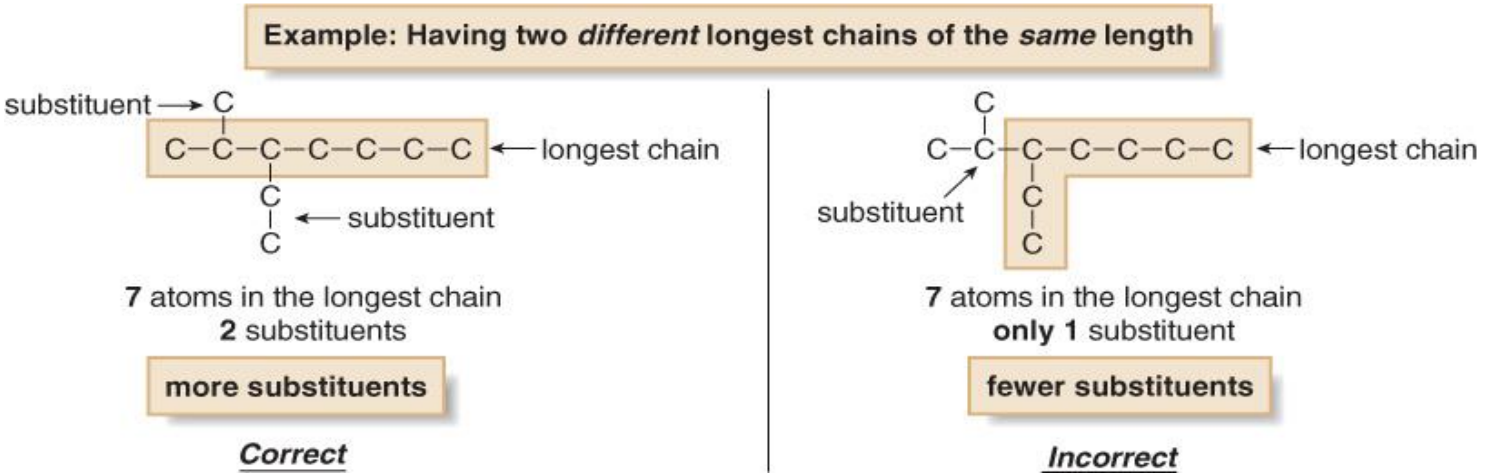
Three- or four-carbon alkyl groups is more complicated because the parent hydrocarbons have more than one type of hydrogen atom. For example, propane has both 1° and 2° H atoms, and removal of each of these H atoms forms a different alkyl group with a different name, propyl or isopropyl.



Alkanes

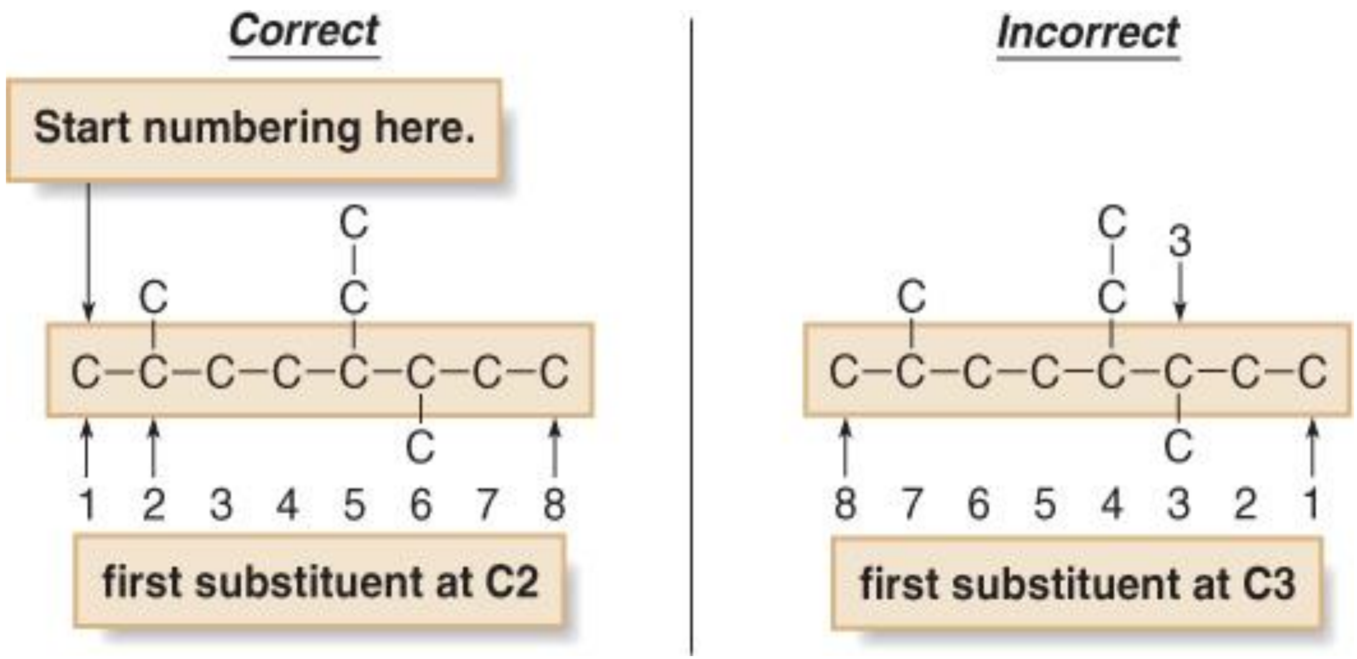
Nomenclature

Also note that if there are two chains of equal length, pick the chain with more substituents. In the following example, two different chains in the same alkane have seven C atoms. We circle the longest continuous chain as shown in the diagram on the left, since this results in the greater number of substituents.



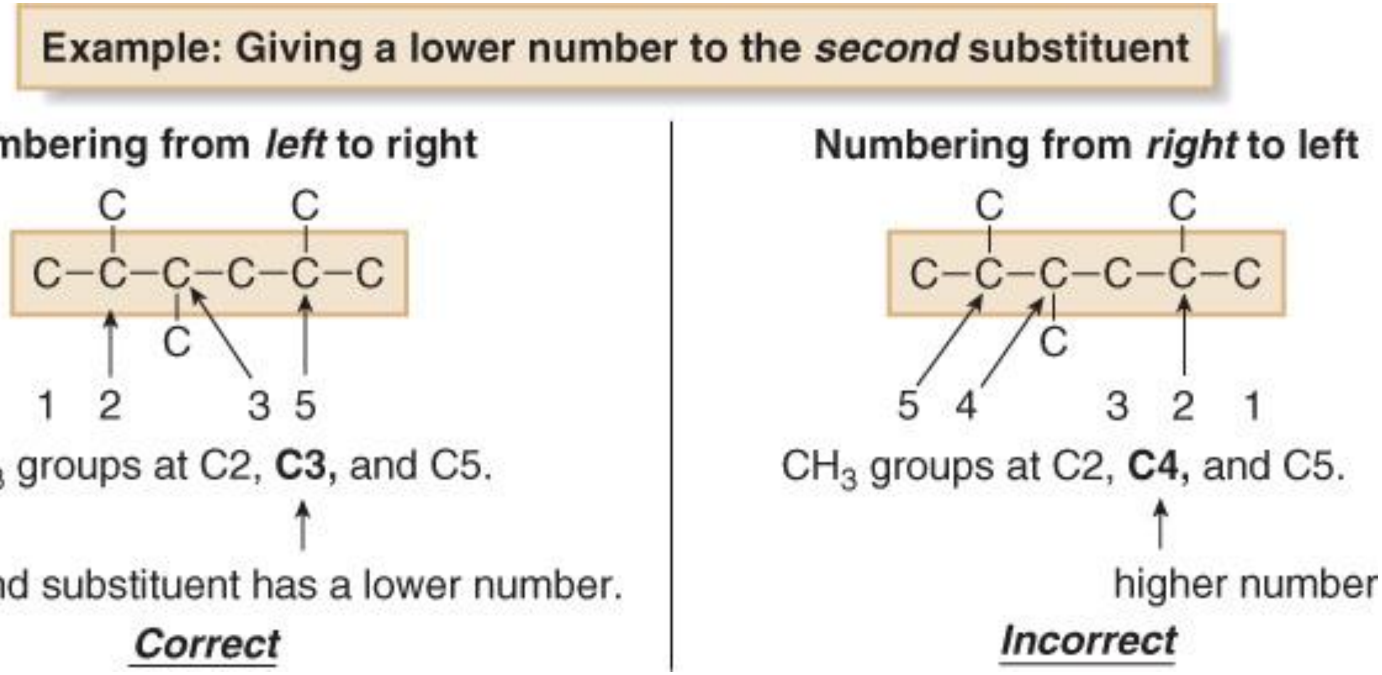
Nomenclature

Number of atoms in the carbon chain to give the first substituent the lowest number.



Nomenclature

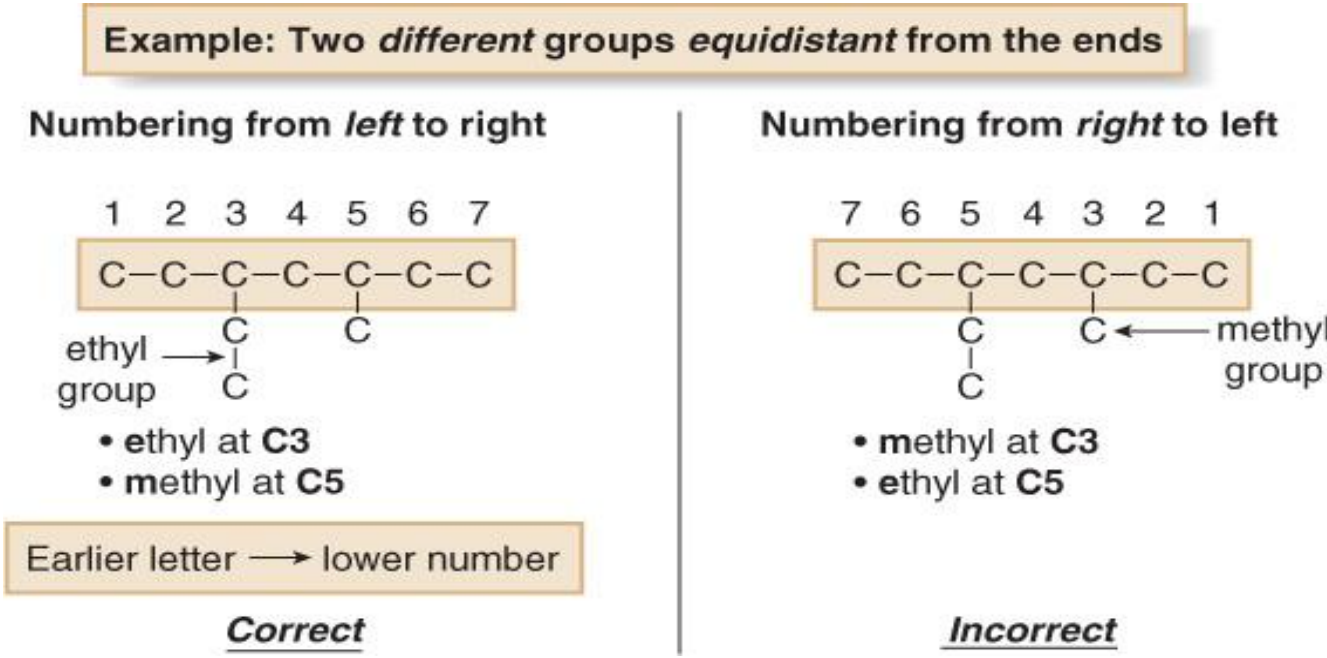
If the first substituent is the same distance from both ends, number of the chain to give the second substituent the lower number.



Alkanes

Nomenclature

When numbering a carbon chain results in the same numbers from either end of the chain, assign the lower number alphabetically to the first substituent.



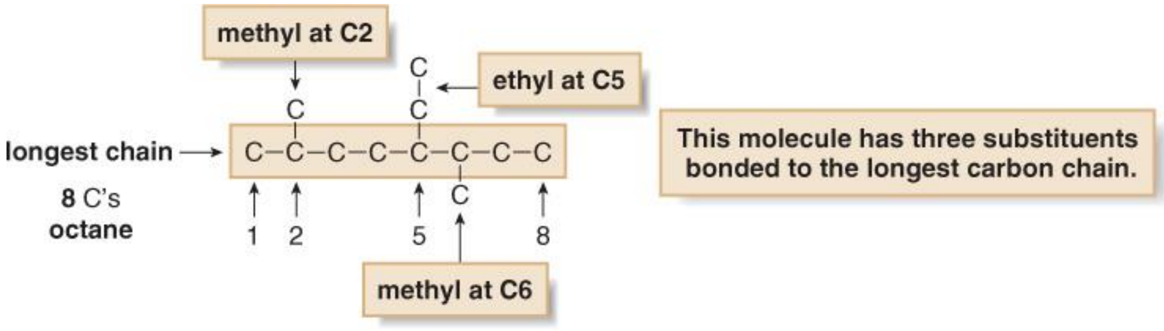
3-ethyl-5-methylheptane

Alkanes

Nomenclature

3. Name and number of the substituents.

- Name the substituents as alkyl groups.
- Every carbon belongs to either the longest chain or a substituent, not both.
- Each substituent needs its own number.
- If two or more identical substituents are bonded to the longest chain, use prefixes to indicate how many: di- for two groups, tri- for three groups, tetra- for four groups, and so forth.



5-ethyl-2,6-dimethyloctane

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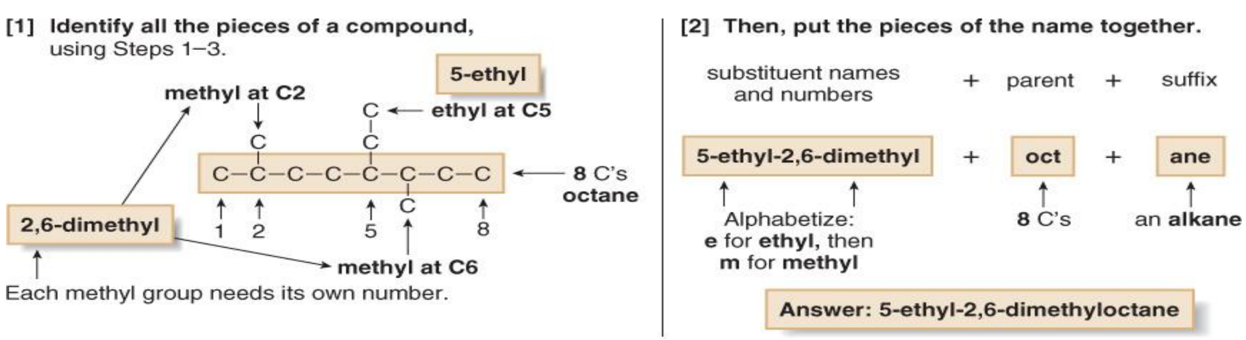
Nomenclature

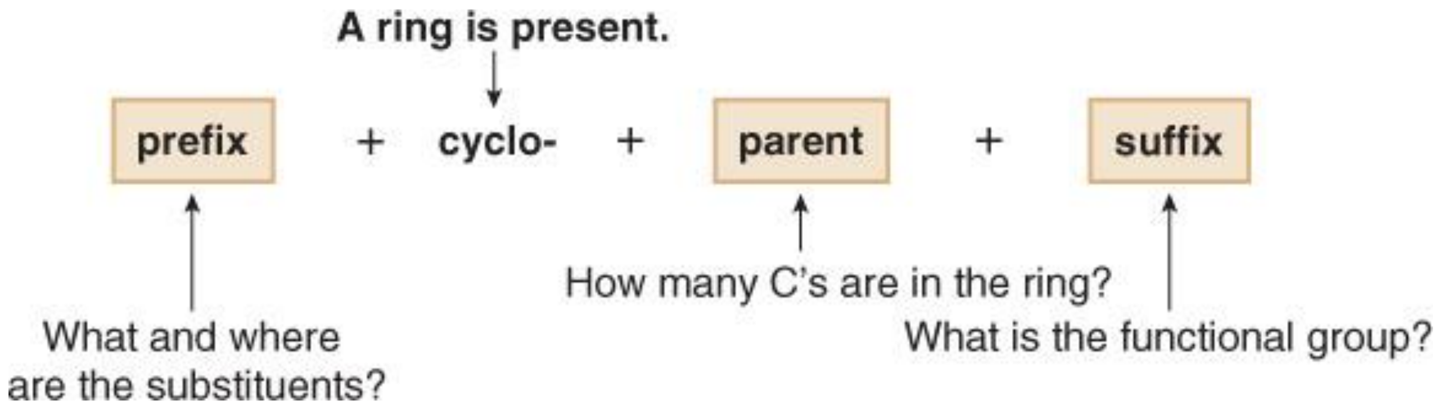
4. Combine substituent names and numbers + parent and suffix.

- Precede the name of the parent by the names of the substituents.
- Alphabetize the names of the substituents, ignoring all prefixes except iso, as in isopropyl and isobutyl.
- Precede the name of each substituent by the number that indicates its location.
- Separate numbers by commas and separate numbers from letters by hyphens. The name of an alkane is a single word, with no spaces after hyphens and commas.

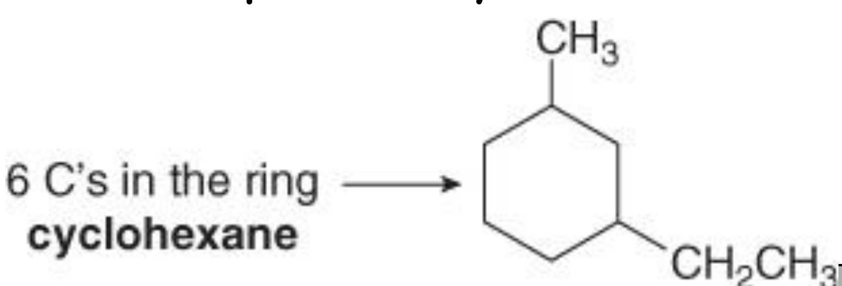


Nomenclature

Cycloalkanes are named by using similar rules, but the prefix cyclo- immediately precedes the name of the parent.



1. Find the parent cycloalkane.

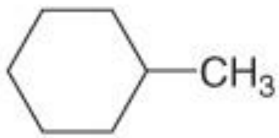


1-ethyl-3-methylcyclohexane

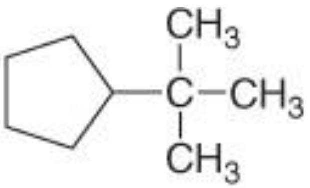
Alkanes

Nomenclature

2. Name and number the substituents. No number is needed to indicate the location of a single substituent.



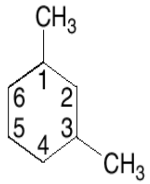
methylcyclohexane



tert-butylcyclopentane

For rings with more than one substituent, begin numbering at one substituent and proceed around the ring to give the second substituent the lowest number.

numbering clockwise

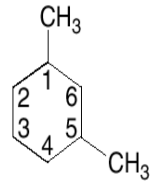


CH_3 groups at C1 and **C3**

The 2nd substituent has a lower number.

Correct: **1,3-dimethylcyclohexane**

numbering counterclockwise



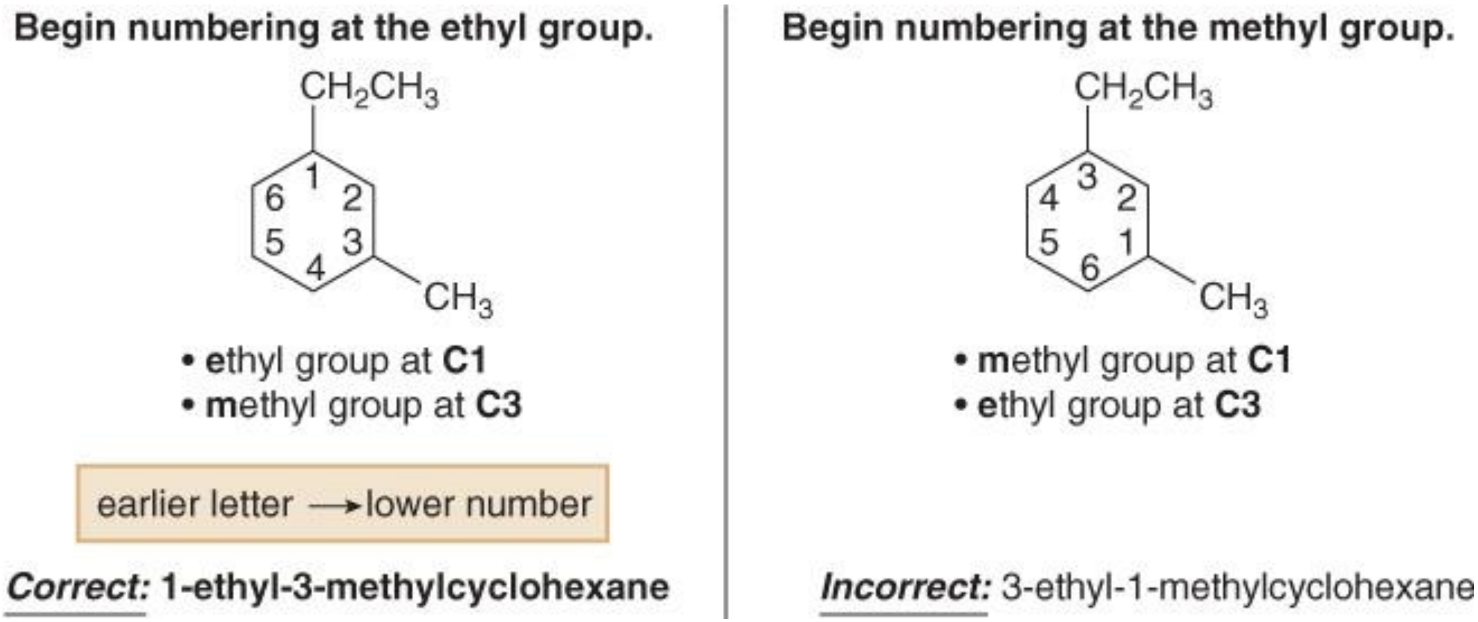
CH_3 groups at C1 and **C5**

Incorrect: 1,5-dimethylcyclohexane

Alkanes

Nomenclature

With two different substituents, number the ring to assign the lower number to the substituents alphabetically.



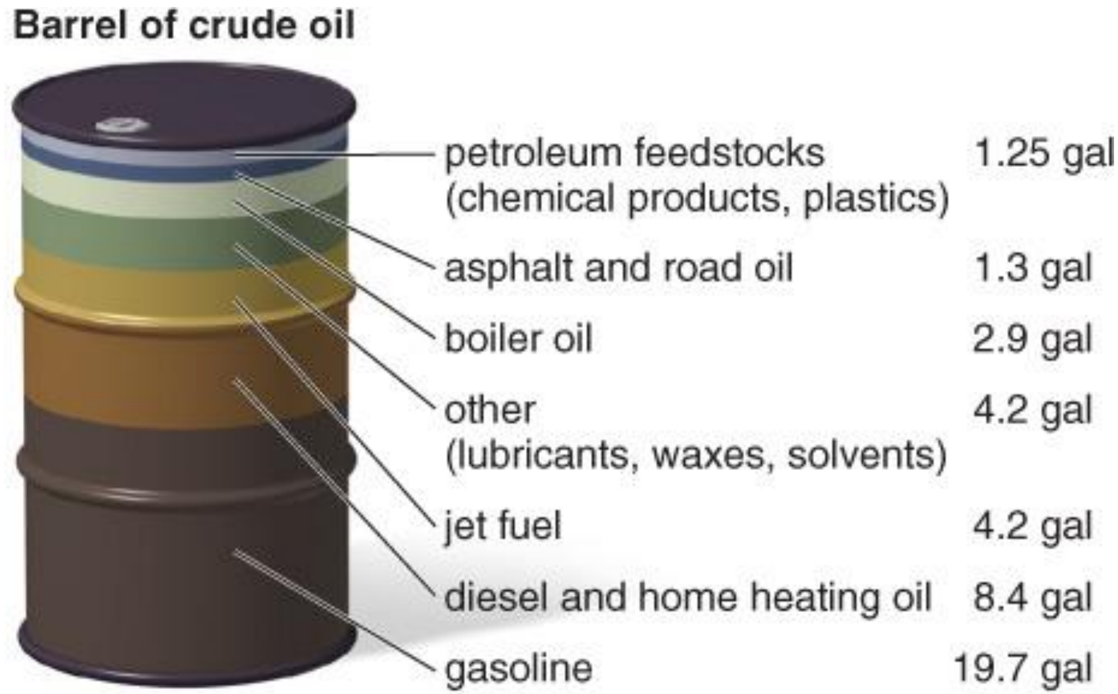
Note the special case of an alkane composed of both a ring and a long chain. If the number of carbons in the ring is greater than or equal to the number of carbons in the longest chain, the compound is named as a cycloalkane.

Alkanes

Industrial Applicants

Many alkanes occur in nature, primarily in natural gas and petroleum.

Natural gas is composed largely of methane, with lesser amounts of ethane, propane and butane.



Petroleum is a complex mixture of compounds, most of which are hydrocarbons containing one to forty carbon atoms. Distilling crude petroleum (called refining), separates it into usable fractions that differ in boiling point.

gasoline: C_5H_{12}—$C_{12}H_{26}$

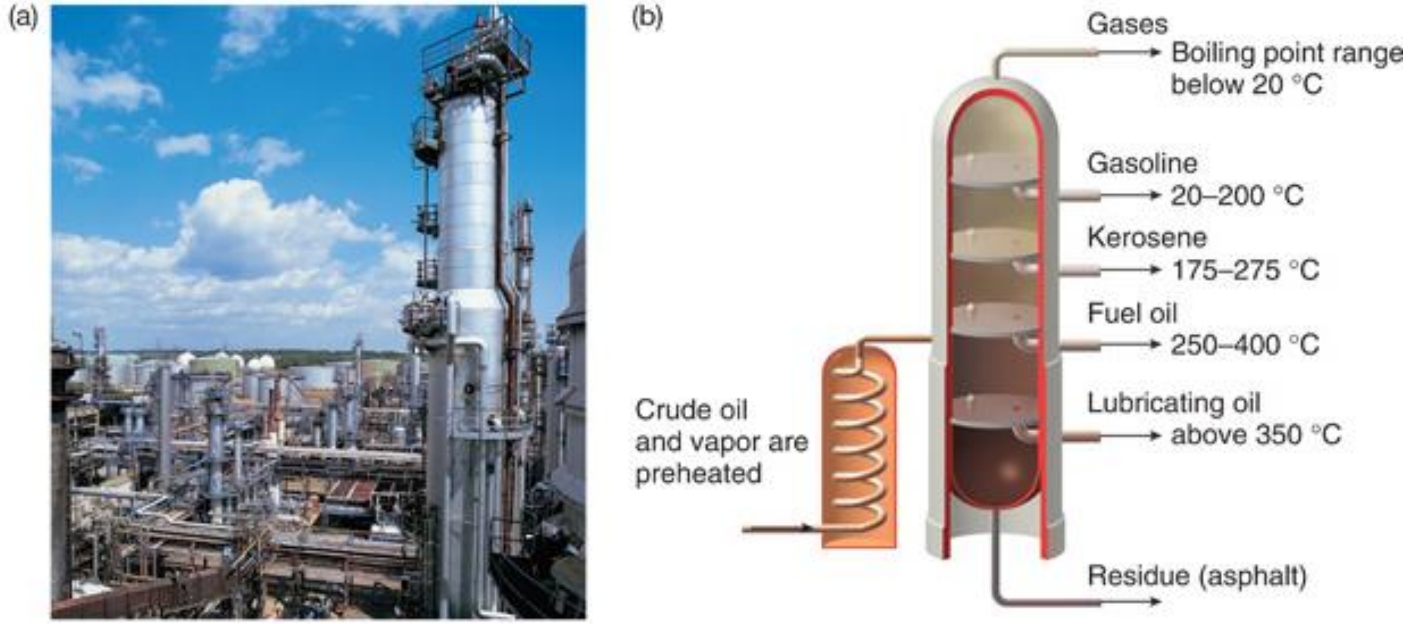
kerosene: $C_{12}H_{26}$—$C_{16}H_{34}$

diesel fuel: $C_{15}H_{32}$—$C_{18}H_{38}$

Alkanes—An Introduction

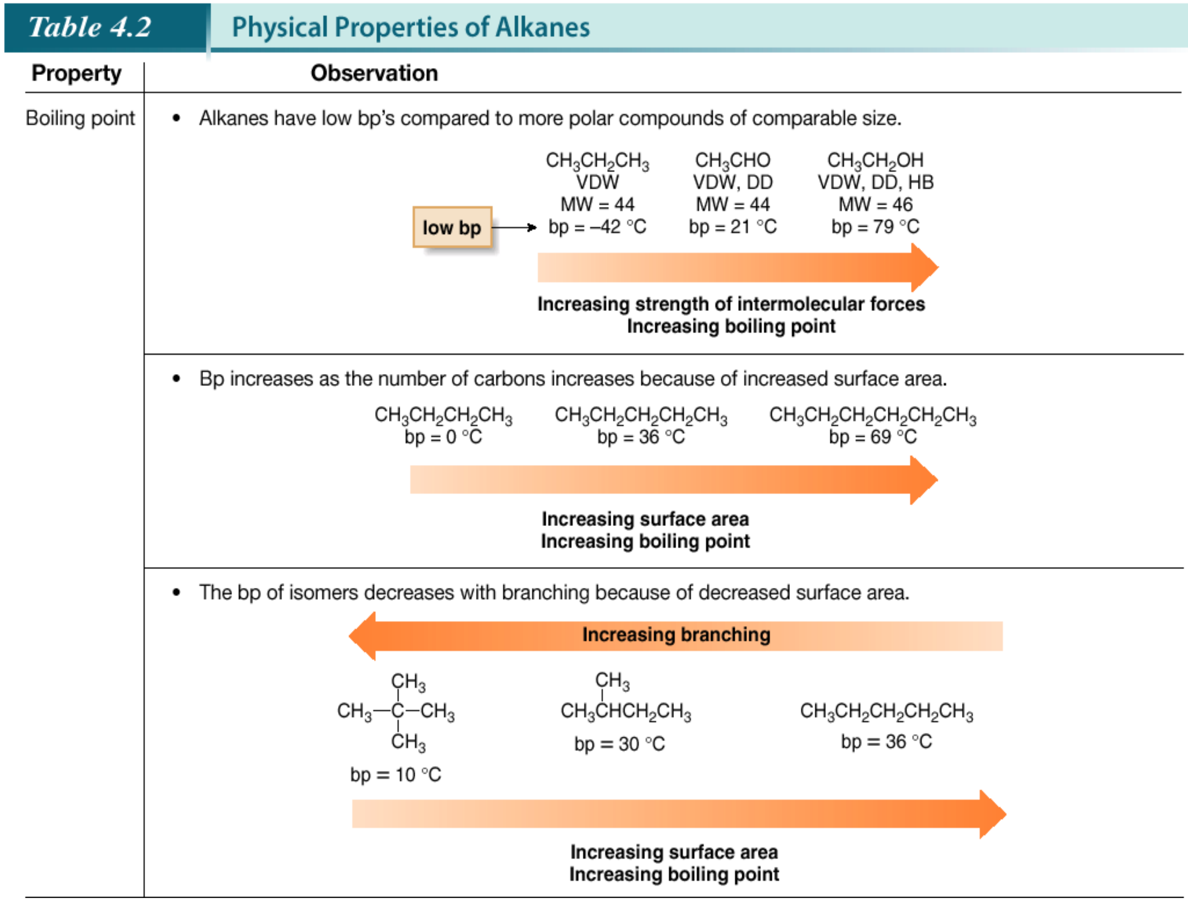
Fossil Fuels:

Figure 4.5 Refining crude petroleum into usable fuel and other petroleum products. (a) An oil refinery. At an oil refinery, crude petroleum is separated into fractions of similar boiling point by the process of distillation. (b) Schematic of a refinery tower. As crude petroleum is heated, the lower-boiling, more volatile components distill first, followed by fractions of progressively higher boiling point.



Alkanes

Physical Properties of Alkanes



Alkanes

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Physical Properties of Alkanes:

Property	Observation
Melting point	• Alkanes have low mp's compared to more polar compounds of comparable size. $CH_3CH_2CH_3$ VDW mp = −190 °C (low mp); CH_3CHO VDW, DD mp = −121 °C **Increasing strength of intermolecular forces** **Increasing melting point**
	• Mp increases as the number of carbons increases because of increased surface area. $CH_3CH_2CH_2CH_3$ mp = −138 °C; $CH_3CH_2CH_2CH_2CH_2CH_3$ mp = −95 °C **Increasing surface area** **Increasing melting point**
	• Mp increases with increased symmetry. $CH_3CH_2CH(CH_3)_2$ mp = −160 °C; $(CH_3)_4C$ mp = −17 °C **Increasing symmetry** **Increasing melting point**
Solubility	• Alkanes are soluble in organic solvents. • Alkanes are insoluble in water.

Key: bp = boiling point; mp = melting point; VDW = van der Waals; DD = dipole–dipole; HB = hydrogen bonding; MW = molecular weight

Conclusion of The Chapter

- Conclusion #1
  - The fundamental of alkanes with its nomenclature were understandable.
- Conclusion #2
  - The fundamental of alkanes included its reactions involves were practically explained.
- Conclusion #3
  - The fundamental of alkanes was practically shown in industrial application especially in petroleum distillation and refining.

Co-author Information

Nurlin Abu Samah is an analytical chemistry lecturer since 2010 and currently she further her PhD study in Universitat Autonoma de Barcelona, Spain. She was graduated from Universiti Kebangsaan Malaysia for her Master of Science in Chemistry. During her undergraduate, she was studied in Universiti Sains Malaysia, Penang.

nurlin@ump.edu.my