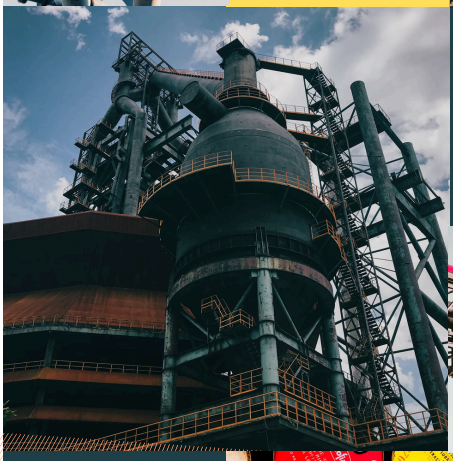

FIRST EDITION

CHEMISTRY OF PETROCHEMICAL PROCESSES VOL. 1

Donald Anak Juan | Nuraiman Bin Abd Rahman | Hafizah Binti Naihi |

Authors

DONALD ANAK JUAN
NURAIMAN BIN ABD RAHMAN
HAFIZAH BINTI NAIHI

POLITEKNIK KUCHING SARAWAK
MINISTRY OF HIGHER EDUCATION
KM22, JALAN MATANG,
93050 KUCHING, SARAWAK.

Phone No. : (082) 845596/7/8
Fax No. : (082) 845023
E-mail : poliku.info@poliku.edu.my
Website : http://www.poliku.edu.my/

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For more information, contact :

Donald Anak Juan
donald_juan@poliku.edu.my

Nuraiman bin Abd Rahman
nuraiman@poliku.edu.my

Hafizah binti Naihi
hafizahnaihi@poliku.edu.my

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HAK CIPTA TERPELIHARA DAN PENAFIAN

HAK CIPTA TERPELIHARA

Tidak dibenarkan mengeluarkan mana-mana bahagian sama ada artikel, ilustrasi dan isi kandungan E-Book ini dalam apa jua bentuk dan dengan apa cara sekalipun, sama ada secara elektronik, fotokopi, rakaman atau cara lain sebelum mendapat izin bertulis daripada Donald Anak Juan, Nuraiman bin Abd Rahman, and Hafizah binti Naihi.

Tanggungjawab hakcipta tidak ada kena mengena dengan maklumat di dalam E-Book ini. Penulis tidak bertanggungjawab ke atas sebarang kesilapan ataupun maklumat yang tidak dimasukkan walaupun langkah berjaga-jaga sudah diambil.

PENAFIAN

Penerbitan ini mengandungi pandangan serta pengalaman penulis dan juga sumber dari yang boleh dipercayai. Ia bertujuan membantu dan menyediakan maklumat berkenaan perkara yang dibincangkan. Penulis tidak bertanggungjawab ke atas mana-mana kerugian, kehilangan atau risiko yang ditanggung oleh perseorangan atau sebagainya, yang timbul akibat daripada penggunaan mana-mana kandungan E-Book ini sama ada secara langsung ataupun tidak langsung.

INTRODUCTION

SYNOPSIS

This e-Book revolves around chemistry in hydrocarbon compounds namely alkanes and alkenes in the petrochemical industry in particular and the chemical, petroleum and process industries in general.

E-Book users will be exposed to the characteristics, uses, reactions and processes that occur for alkanes and alkenes in the petrochemical industry. Through this e-Book, users can not only understand and master alkanes and alkenes but they can also apply the knowledge they gain in their daily lives..

SINOPSIS

e-Book ini berkisarkan kepada kimia dalam sebatian hidrokarbon iaitu alkana dan alkena dalam industri petrokimia khususnya dan industri kimia, petroleum dan proses secara amnya.

Pengguna e-Book akan didedahkan dengan ciri-ciri, kegunaan, tindak balas serta proses-proses yang berlaku untuk alkana dan alkena di dalam industri petrokimia. Melalui e-Book ini, pengguna bukan sahaja dapat memahami serta menguasai alkana dan alkena malah mereka juga dapat mengaplikasikan pengetahuan yang mereka peroleh di dalam kehidupan seharian.

Donald Anak Juan

AUTHOR'S PROFILE

Authors background

The author is a graduate engineer (IEM), background of Chemical and Process Engineering before further studies in Chemical Engineering (Bioprocess). The author also has four years of industrial working experiences in one of Malaysia's leading petrochemical company.

Education

2004-2007

UITM SARAWAK

Diploma in Science (Biology and Chemistry)

2007-2011

UITM SHAH ALAM

Bachelor of Engineering (Hons.) Chemical and Process

2019-2021

UNIVERSITI KEBANGSAAN MALAYSIA

Master of Engineering (Chemical) - Bioprocess

Contact

019-8066707

donald_juan@poliku.edu.my

Politeknik Kuching Sarawak

Experience

Lecturer, 2015-Present

- Appointed as a Lecturer of Diploma in Process Engineering (Petrochemical), Politeknik Kuching Sarawak since 2015.
- Manage portfolio such as Pengerusi Kurikulum DPE (2022-present), Penyelaras YES (2022-present), Penyelaras Latihan Staf (2022-present), Penyelaras Akreditasi (2022-2023) and Penyelaras CQI (2022-2023).
- Responsible as the course coordinator for courses such as Chemistry of Petrochemical Processes (2021 - present), Piping and Instrumentation Diagram (2015-2019), and Heat Transfer (2016-2017).
- Teach other courses such as Applied Chemistry, Process Engineering Lab 2 & 3, and Final Year Project (Project 1 & 2).

Nuraiman bin Abd Rahman

AUTHOR'S PROFILE

Authors background

The author hold a Bachelor of Chemical Technology, with a qualification on ensuring operational safety and regulatory compliance, he have experience in implementing and optimizing safety protocols within the department. In parallel, he have cultivated a dynamic skill set in software development over the past four years. This skills in software has enabled him to bridge technical knowledge with background in chemical technology and safety.

Education

2012-2015

UNIVERSITI KEBANGSAAN MALAYSIA

Bachelor of Chemical Technology

Contact

012-3361213

nuraiman@poliku.edu.my

1Politeknik Kuching Sarawak

Experience

Lecturer, 2020-Present

- Appointed as a Diploma in Process Engineering (Petrochemical) (DPE) Lecturer, Politeknik Kuching Sarawak in 2020.
- Manage portfolios such as Safety and Health Coordinator (DPE) (2021-2022), and Chemistry Lab Supervisor (2020-present).
- Teach courses such as Applied Chemistry, Chemistry Lab and Chemistry of Petrochemical Processes.

Hafizah binti Naihi

AUTHOR'S PROFILE

Authors background

The author is a graduate engineer (BEM) with a background in Chemical Engineering. The author also has three and a half years of industrial working experience in manufacturing.

Education

2007-2011
UNIVERSITI PUTRA MALAYSIA
Bachelor of Engineering (Chemical)

2020-2023
UNIVERSITI MALAYSIA SARAWAK
Master of Engineering (Chemical)

Experience

Lecturer, 2015-Present

- Appointed as a Diploma in Process Engineering (Petrochemical) (DPE) Lecturer, Politeknik Kuching Sarawak in 2015.
- Manage portfolios such as Head of Programme (DPE) (2024-present), and Student Project Coordinator (2015-2024).
- Teach courses such as Petrochemical Production Processes, Mass and Energy Balance, Thermodynamics, Wastewater Engineering, and Utility Plant.

Contact

010-9768536

hafizahnaihi@poliku.edu.my

1Politeknik Kuching Sarawak

TABLE OF CONTENTS

Chapter 1

Paraffinic Hydrocarbons

INTRODUCTION OF PARAFFINIC HYDROCARBONS

- Natural gas and petroleum contain a large amount of paraffin.
- Paraffinic hydrocarbons are better known as alkanes.
- Any of the saturated hydrocarbons with the general formula CnH2n+2, where C is a carbon atom, H is a hydrogen atom, and n is an integer, is referred to as a paraffin hydrocarbon.
- Paraffins containing fewer than 5 carbon atoms per molecule are usually gaseous at room temperature, those having 5 to 15 carbon atoms are usually liquids, and the straight-chain paraffins having more than 15 carbon atoms per molecule are solids.
- Branched-chain paraffins have a much higher octane number rating than straight-chain paraffins and, therefore, are the more desirable constituents of gasoline.

CLASSIFICATION OF HYDROCARBONS

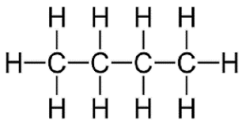
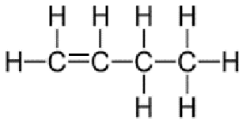
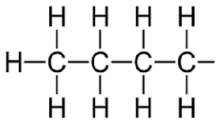
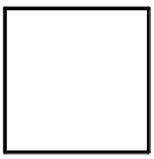
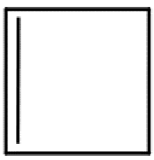
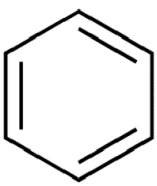
Type of Compound	General Formula	Example
Alkane	C_nH_{2n+2}	
Alkene	C_nH_{2n-2}	
Alkyl	C_nH_{2n+1}	
Cycloalkene	C_nH_{2n}	
Cycloalkene	C_nH_{2n-2}	
Benzene (aromatic compound)	–	

Figure 1.1: Classification of hydrocarbon

PARAFFINIC HYDROCARBONS (ALKANES)

- Paraffinic hydrocarbons are subdivided into the following three groups such as the linear straight-chain alkanes, branched alkanes, and cycloalkanes.
- Paraffinic hydrocarbons are also refer as saturated hydrocarbons.
- It is the simplest and least reactive hydrocarbon species containing only carbons and hydrogens.
- They are commercially very important, being the principal constituent of gasoline and lubricating oils and are extensively employed in organic chemistry.
- Paraffinic hydrocarbons are the role of pure alkanes such as hexane which is delegated mostly to solvents.
- The distinguishing feature of an alkane, making it distinct from other compounds that also exclusively contain carbon and hydrogen, is its lack of unsaturation.

ALKANES

- General formula for alkanes is CnH2n+2 where n is the number of carbon atoms n the molecule. Alkanes name ending with –ane.

- Methane (CH4) is the first member of this family. If you swap out one hydrogen atom from methane for a carbon atom and connect the necessary amount of hydrogens, you get C2H6.

- Ethane is the name given to this hydrocarbon, which has the chemical formula C2H6.

- Therefore, you may think of C2H6 as being formed from CH4 by substituting a -CH3 group for one hydrogen atom.

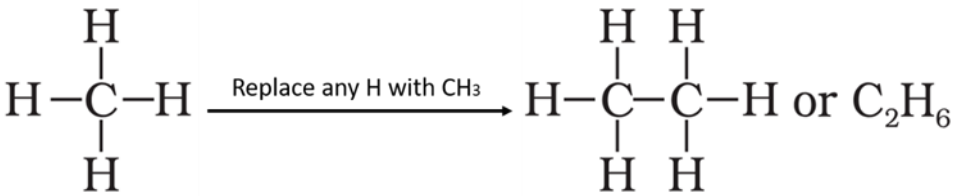


Figure 1.2: The formation of ethane from ethane

ALKANES

- That is to say, it contains no double or triple bonds, which are highly reactive in organic chemistry.
- Though not totally devoid of reactivity, their lack of reactivity under most laboratory conditions makes them a relatively uninteresting, though very important component of organic chemistry.
- As with other organic compounds, the carbon atoms in alkanes may form straight chains, branched chains, or rings.
- These three kinds of alkanes are straight chain alkanes, branched chain alkanes and cycloalkane.
- When an alkane having hydrogen is removed from one bond, it is called an alkyl group.
- This Alkyl group is often denoted by the letter R the same as halogens represent by the letter X.

ALKANES

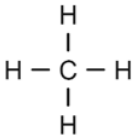
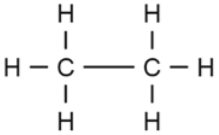
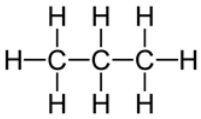
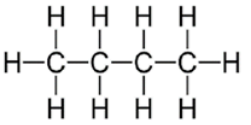
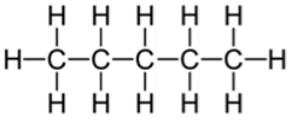
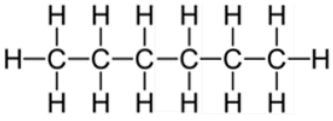
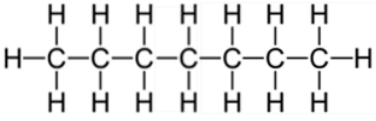
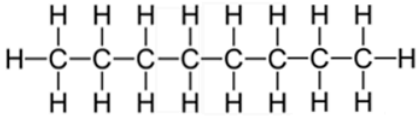
Type of Compound	General Formula	Example
Methane	CH_4	
Ethane	C_2H_6	
Propane	C_3H_8	
Butane	C_4H_{10}	
Pentane	C_5H_{12}	
Hexane	C_6H_{14}	
Heptane	C_7H_{16}	
Octane	C_8H_{18}	

Figure 1.3: List of the first 8 alkanes

ALKYL

- If you imagine removing hydrogen atom from an alkane, the partial structure that remains is called an alkyl group.

- Alkyl group are not stable compounds themselves, they simply parts of larger compounds.

- Alkyl groups are named by replacing the –ane ending of the parent alkane with an –yl ending.

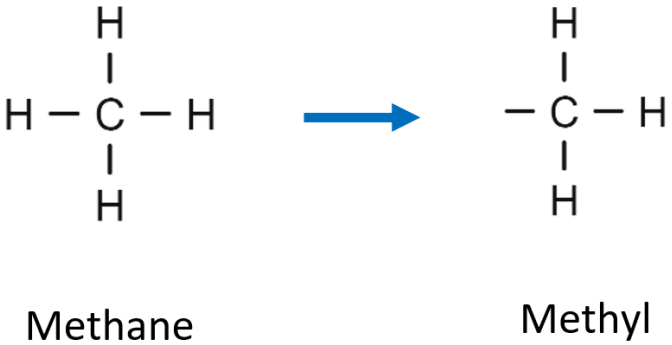


Figure 1.4: The formation methyl from methane

NAMING ALKANE

- Naming of an alkane involves three main steps. Start from finding the longest carbon chain, number the carbon chain with the most substituents and the lowest number at each substituent and lastly identify the type of substituents.

- When naming alkane, three basic formats can be used. Alkane with one substituent, two same substituents and two different substituents.

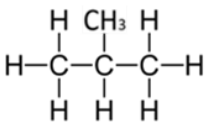
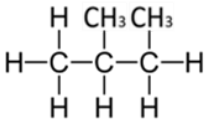
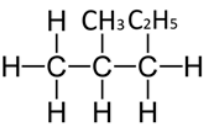
Type of substituent	Format	Example
One substituent	no.–subs longest C	 2–methylpropane
Two same substituents	no., no.–prefix subs longest C	 1, 2–dimethylpropane
Two different substituents	no.–subs–no.–subs longest C	 1–ethyl–2–methylpropane

Figure 1.5: Type of substituent for alkane

ONE SUBSTITUENT ALKANE

- The simplest type of chemical structure is an alkane with a single substituent since there is only one substituent attached to the parent structure.
- To name an alkane with a single substituent, follow the steps below:

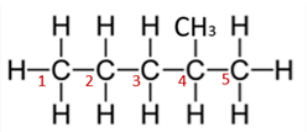
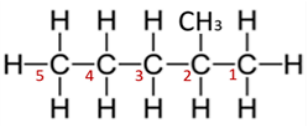
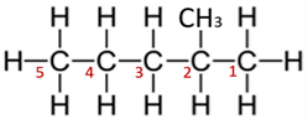
Step	Format	Example
1	no.–subs **longest C** • use **one substituent** format • find the longest carbon chain (C = 5) • 5 carbon is pentane	 no.–subs**pentane**
2	**no.**–subs longest C • number the carbon chain with the most substituents and the lowest number at each substituent • substituent at C_2	 **2**–subspentane
3	no.–**subs** longest C • identify the type of substituent • CH_3 is methyl	 2–**methyl**pentane

Figure 1.6: Steps in naming one substituent alkane

TWO SAME SUBSTITUENT ALKANE

- Two same substituent alkane indicate that the chemical structure attached with two identical substituents.
- Therefore, prefix need to be used that is **di** for 2 and **tri** for 3 same substituents.
- To name an alkane with two same substituents, follow the steps below:

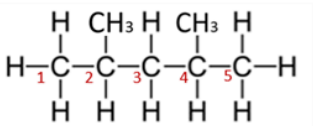
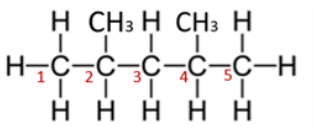
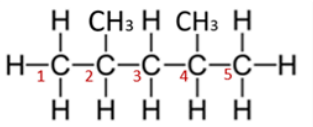
Step	Format	Example
1	no., no.– prefix subs **longest C** • use **two same substituents** format • find the longest carbon chain (C = 5) • 5 carbon is pentane	 no., no.–prefix subs **pentane**
2	**no., no.**– prefix subs longest C • number the carbon chain with the most substituents and the lowest number at each substituent • substituent at C_2 & C_4	 **2, 4**–prefix subs pentane
3	no., no.– **prefix subs** longest C • identify the type of substituent • CH_3 is methyl • prefix for 2 methyl is **di**	 2, 4– dimethylpentane

Figure 1.7: Steps in naming two same substituent alkane

TWO DIFFERENT SUBSTITUENT ALKANE

- Two different substituent alkane indicate that the chemical structure attached with two different substituents.
- Therefore, two different number need to be placed in front of substituents name.
- To name an alkane with two different substituents, follow the steps below:

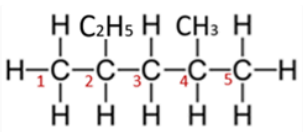
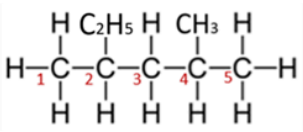
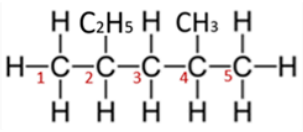
Step	Format	Example
1	no. – subs – no. – subs **longest C** • use **two different substituents** format • find the longest carbon chain (C = 5) • 5 carbon is pentane	 no.–subs–no.–subs **pentane**
2	**no.**–subs–**no.**–subs **longest C** • number the carbon chain with the most substituents and the lowest number at each substituent • substituent at C_2 & C_4	 **2**–subs–**4**–subs pentane
3	**no.**–subs–**no.**–subs **longest C** • identify the type of substituent • C_2H_5 is ethyl & CH_3 is methyl • Ethyl come first at C_2 then methyl at C_4 are based on alphabetical order **(e then m)**	 2–**ethyl**–4–**methyl**pentane

Figure 1.8: Steps in naming two same substituent alkane

CYCLOALKANES

- Cycloalkanes are also known as alicyclic compounds (aliphatic cyclic). Cycloalkanes consists of rings of –CH2– units.
- The general formula CnH2n and can be represented by polygons in skeletal drawings.
- The general formula CnH2n and can be represented by polygons in skeletal drawings.
- For a ring to become a parent, the number of atoms in the ring must be more than the substituent.

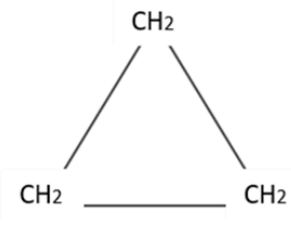
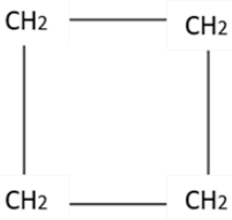
Type of Compound	General Formula	Example
Cyclopropane	C3H6	
Cyclobutane	C4H8	

Figure 1.9: List of cycloalkanes, n= 3 and 4

CYCLOALKANES

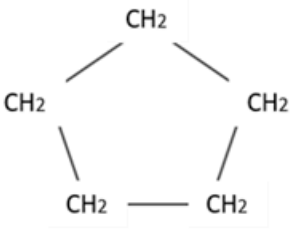
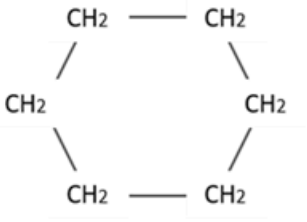
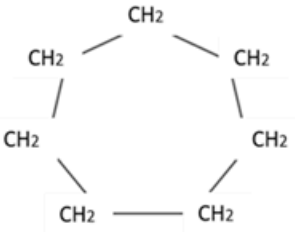
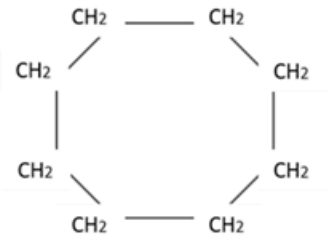
Type of Compound	General Formula	Example
Cyclopentane	C_5H_{10}	
Cyclohexane	C_6H_{12}	
Cycloheptane	C_7H_{14}	
Cyclooctane	C_8H_{16}	

Figure 1.10: List of cycloalkanes, n= 5, 6, 7, and 8

ONE SUBSTITUENT CYCLOALKANE

- The simplest type of chemical structure is an cycloalkane with a single substituent since there is only one substituent attached to the parent structure.
- To name an cycloalkane with a single substituent, follow the steps below:

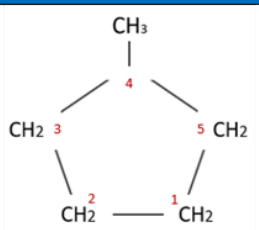
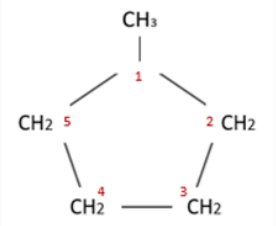
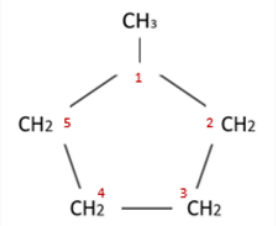
Step	Format	Example
1	no.–subs **longest C** • use **one substituent** format • find the longest carbon chain (C = 5) • 5 carbon is cyclopentane	 no.–subs**cyclopentane**
2	**no.**–subs longest C • number the carbon chain with the most substituents and the lowest number at each substituent • substituent at C_1	 **1**–subscyclopentane
3	no.–**subs** longest C • identify the type of substituent • CH_3 is methyl	 1–**methyl**cyclopentane or **methyl**cyclopentane

Figure 1.11: Steps in naming one substituent cycloalkane

TWO SAME SUBSTITUENT CYCLOALKANE

- Two same substituent cycloalkane indicate that the chemical structure attached with two identical substituents.
- Therefore, prefix need to be used that is **di** for 2 and **tri** for 3 same substituents.
- To name an cycloalkane with two same substituents, follow the steps below:

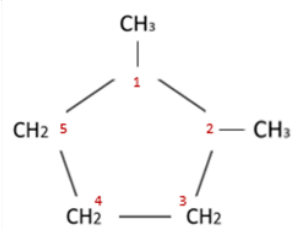
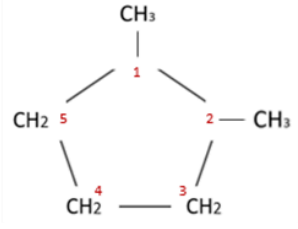
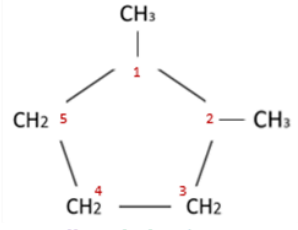
Step	Format	Example
1	no., no.–prefix subs **longest C** • use **two same substituents** format • find the longest carbon chain (C = 5) • 5 carbon is cyclopentane	 no., no.–prefix subs **cyclopentane**
2	**no., no.**–prefix subs longest C • number the carbon chain with the most substituents and the lowest number at each substituent • substituent at C_1 & C_2	 **1, 2**–prefix subs cyclopentane
3	no., no.–**prefix subs** longest C • identify the type of substituent • CH_3 is methyl • prefix for 2 methyl is **di**	 2, 4–**dimethyl**cyclopentane

Figure 1.12: Steps in naming two same substituent cycloalkane

TWO DIFFERENT SUBSTITUENT CYCLOALKANE

- Two different substituent cycloalkane indicate that the chemical structure attached with two different substituents.
- Therefore, two different number need to be placed in front of substituents name.
- To name an cycloalkane with two different substituents, follow the steps below:

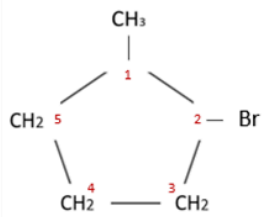
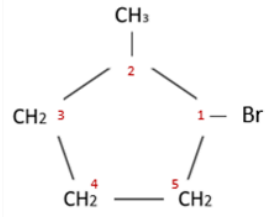
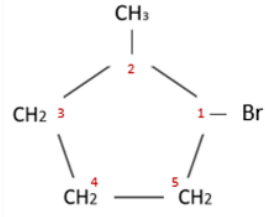
Step	Format	Example
1	no.–subs–no.–subs **longest C** • use **two different substituents** format • find the longest carbon chain (C = 5) • 5 carbon is cyclopentane	 no.–subs–no.–subs **cyclopentane**
2	**no.**–subs–**no.**–subs **longest C** • number the carbon chain with the most substituents and the lowest number at each substituent • substituent at (C = 1) & (C = 2)	 **1**–subs–**2**–subscyclopentane
3	**no.**–subs–**no.**–subs **longest C** • identify the type of substituent • (Br = bromine) & (CH_3 = methyl) • bromine come first (C = 1) then methyl (C = 2) are based on alphabetical order **(b then m)**	 1–**bromo**–2–**methyl**cyclopentane

Figure 1.13: Steps in naming two different substituent alkane

PHYSICAL CHARACTERISTICSS OF ALKANES

- The physical characteristics of alkanes discussed in this Figure 1.14 are boiling point, melting point, density, conductivity, and solubi are boiling point, melting point, density, conductivity, and solubility.

Alkane	Formula	Physical State at 25°C	Boiling Point (°C)	Melting Point (°C)	Density (g/cm³ at 20°C)	Electrical Conductivity	Solubility in Water
Methane	CH_4	Gas	-161.5	-182.5	0.000668	Non-conductor	Insoluble
Ethane	C_2H_6	Gas	-88.6	-172.0	0.001261	Non-conductor	Insoluble
Propane	C_3H_8	Gas	-42.1	-187.7	0.002009	Non-conductor	Insoluble
Butane	C_4H_{10}	Gas	-0.5	-138.4	0.002493	Non-conductor	Insoluble
Pentane	C_5H_{12}	Liquid	36.1	-129.7	0.626	Non-conductor	Insoluble
Hexane	C_6H_{14}	Liquid	68.7	-95.3	0.660	Non-conductor	Insoluble
Heptane	C_7H_{16}	Liquid	98.4	-90.6	0.684	Non-conductor	Insoluble
Octane	C_8H_{18}	Liquid	125.7	-57.8	0.703	Non-conductor	Insoluble
Nonane	C_9H_{20}	Liquid	150.8	-51.6	0.718	Non-conductor	Insoluble
Decane	$C_{10}H_{22}$	Liquid	174.1	-29.7	0.730	Non-conductor	Insoluble

Figure 1.14: Physical characteristics of alkanes

PHYSICAL CHARACTERISTICSS OF ALKANES

- Solubility in water
  Due to very little difference of electronegativity between carbon and hydrogen and covalent nature of C-C bond or C-H bond, alkanes are generally non-polar molecules.

- All paraffins are colourless.

- Boiling point of paraffinic hydrocarbons
  As the intermolecular Van Der Waals forces increase with the increase of the molecular size or the surface area of the molecule.

  The boiling point of alkanes increases with increasing molecular weight. The straight-boiling point in comparison to their structural isomers.

CHEMICAL CHARACTERISTICS OF ALKANES

- Figure 1.15 below elaborates on three important chemical reactions of alkanes such as Combustion Reaction, Halogenation Reaction, and Cracking Reaction.

Reaction Type	Chemical Reaction Example	Chemicals Involved	Reaction Steps	Applications
Combustion (Complete)	$CH_4+2O_2 \rightarrow CO_2+2H_2O$	Methane (CH_4), Oxygen (O_2), Carbon Dioxide (CO_2), Water (H_2O)	▪ Highly exothermic reaction ▪ Produces carbon dioxide and water vapor ▪ Complete oxidation in the presence of sufficient oxygen	Energy production, heating
Combustion (Incomplete)	$CH_4+O_2 \rightarrow CO+2H_2O$	Methane (CH_4), Oxygen (O_2), Carbon Monoxide (CO), Water (H_2O)	▪ Occurs with limited oxygen supply ▪ Produces carbon monoxide and water vapor ▪ Less energy released compared to complete combustion	Industrial processes, fuel efficiency
Halogenation (Fluorine)	$CH_4+F_2 \rightarrow CH_3F+HF$	Methane (CH_4), Fluorine (F_2), Tetrafluoromethane (CF_4), Hydrofluoric Acid (HF)	▪ Initiation: $F_2 \rightarrow 2F\cdot$ ▪ Propagation: $F\cdot+CH_4 \rightarrow CH_3\cdot+HF$ $CH_3\cdot+F_2 \rightarrow CH_3I+F\cdot$ ▪ Termination: $CH_3\cdot+F\cdot \rightarrow CH_3F$ $F\cdot+F\cdot \rightarrow F_2$	Pharmaceuticals, materials science

Figure 1.15: Chemical characteristics properties of alkanes

CHEMICAL PROPERTIES OF ALKANES

Reaction Type	Chemical Reaction Example	Chemicals Involved	Reaction Steps	Applications
Halogenation (Iodine)	$CH_4+I_2 \rightarrow CH_3I+HI$	Methane (CH_4), Iodine (I_2), Methyl Iodide (CH_3I), Hydroiodic Acid (HI)	▪ Initiation: $I_2 \rightarrow 2I\cdot$ ▪ Propagation: $I\cdot+CH_4 \rightarrow CH_3\cdot+HI$ $CH_3\cdot+ I_2 \rightarrow CH_3I+ I\cdot$ ▪ Termination: $CH_3\cdot+ I\cdot \rightarrow CH_3I$ $I\cdot+I\cdot \rightarrow I_2$	Organic synthesis, chemical modifications
Halogenation (Chlorine)	$CH_4+Cl_2 \rightarrow CH_3Cl+HCl$	Methane (CH_4), Chlorine (Cl_2), Methyl Chloride (CH_3Cl), Hydrochloric Acid (HCl)	▪ Initiation: $Cl_2 \rightarrow 2Cl\cdot$ ▪ Propagation: $Cl\cdot+CH_4 \rightarrow CH_3\cdot+HCl$ $CH_3\cdot+ Cl_2 \rightarrow CH_3Cl+ Cl\cdot$ ▪ Termination: $CH_3\cdot+ Cl\cdot \rightarrow CH_3Cl$ $Cl\cdot+Cl\cdot \rightarrow Cl_2$	Organic synthesis, industrial processes
Halogenation (Bromine)	$CH_4+Br_2 \rightarrow CH_3Br+HBr$	Methane (CH_4), Bromine (Br_2), Methyl Bromide (CH_3Br), Hydrobromic Acid (HBr)	▪ Initiation: $Br_2 \rightarrow 2Br\cdot$ ▪ Propagation: $Br\cdot+CH_4 \rightarrow CH_3\cdot+HBr$ $CH_3\cdot+ Br_2 \rightarrow CH_3Br+ Br\cdot$ ▪ Termination: $CH_3\cdot+ Br\cdot \rightarrow CH_3Br$ $Br\cdot+Br\cdot \rightarrow Br_2$	Organic synthesis, pharmaceuticals
Cracking	$C_{10}H_{22} \rightarrow C_5H_{12}+C_5H_{10}$	Decane ($C_{10}H_{22}$), Various smaller hydrocarbons	▪ Breaks larger hydrocarbon molecules into smaller, more useful molecules ▪ Can be thermal or catalytic ▪ Used in petroleum refining	Petrochemical industry, gasoline production

Figure 1.16: Chemical characteristics of alkanes

CHEMICAL CHARACTERISTICS OF ALKANES

- Alkanes react only very poorly with ionic or other polar substances.
- The pKa values of all alkanes are above 50, and so they are practically inert to acids and bases.
- In crude oil the alkane molecules have remained chemically unchanged for millions of years.
- However redox reactions of alkanes, in particular with oxygen and the halogens, are possible as the carbon atoms are in a strongly reduced condition.
- Reaction with oxygen leads to combustion without any smoke; with halogens, substitution. In addition, alkanes have been shown to interact with, and bind to, certain transition metal complexes.

CHEMICAL CHARACTERISTICS OF ALKANES

- Alkanes free radicals, molecules with unpaired electrons, play a large role in most reactions of alkanes, such as cracking and reformation where long-chain alkanes are converted into shorter-chain alkanes and straight-chain alkanes into branched-chain isomers.

- In highly branched alkanes and cycloalkanes, the bond angles may differ significantly from the optimal value (109.5°) in order to allow the different groups sufficient space.

- This causes a tension in the molecule, known as steric hinderance, and can substantially increase the reactivity.

- The same is preferred for alkenes too.

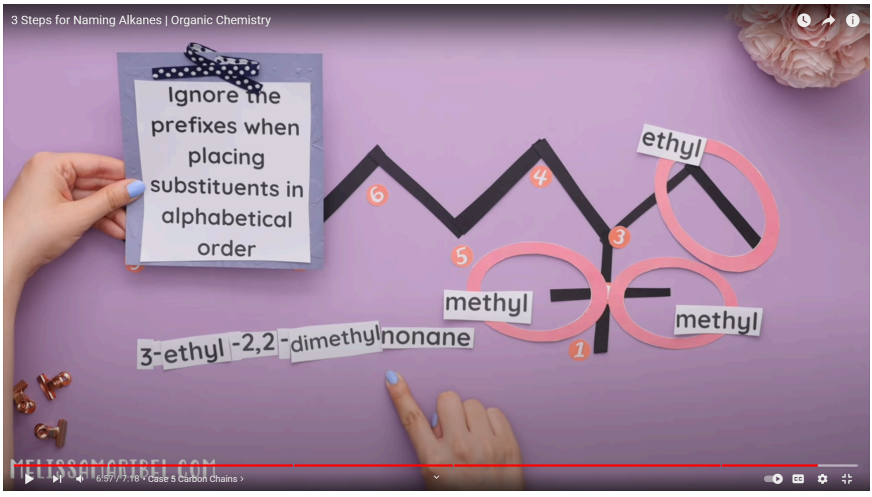
CHEMISTRY OF PETROCHEMICAL PROCESSES, VOL. 1

Chapter 2

Paraffinic Hydrocarbons

Interactive Activities 1

Watch Alkane Tutorial on YouTube



Scan the QR Code above for the alkane interactive video

Class Activity: Naming the alkane

Scan the QR Code above to answer the Quiz

Class Activity: Chemical Properties of the alkane

Scan the QR Code above to answer the Quiz

CHEMISTRY OF PETROCHEMICAL PROCESSES, VOL. 1

Chapter 3

Olefinic Hydrocarbons

INTRODUCTION OF OLEFINIC HYDROCARBONS

- Alkenes, commonly referred to as olefins, are partially unsaturated straight-chain hydrocarbons characterized by one or two double carbon—carbon bonds.

- Olefins are produced at crude oil refineries and petrochemical plants and are not naturally occurring constituents of oil and natural gas.

- In the IUPAC naming system, the name of the olefins suffixes with the “ene”.

- Ethylene is the smallest olefin. The common olefins examples are propane, ethene, butene, and pentene.

- Olefin is a man-made fabric that is extremely durable. The fibres are created using heat, pressure, and a catalyst.

- In fact, olefin often goes by another name: polypropylene. This chemically created fabric is often considered to be more environmentally friendly than cotton, silk, and other natural fibres.

OLEFINIC HYDROCARBONS (ALKENES)

- General formula for alkenes are CnH2n where n is the number of carbon atoms n the molecule.
- Alkenes are relatively stable compounds, but are more reactive than alkanes.
- The olefins most commonly used in the alkylation unit are butylene and propylene to produce alkylate.
- Figure 2.1 below shows the prefix of alkene with number of carbon start from 2.

Number of carbons (n)	Prefix	Alkene (ending-ene)	Alkylene (ending-ylene)	Formula (C_nH_{2n})
1	-	-	-	-
2	Eth	Ethene	Ethylene	C_2H_4
3	Prop	Propene	Propylene	C_3H_6
4	But	Butene	Butylene	C_4H_8
5	Pent	Pentene	Pentylene	C_5H_{10}
6	Hex	Hexene	Hexylene	C_6H_{12}
7	Hept	Heptene	Heptylene	C_7H_{14}
8	Oct	Octene	Octylene	C_8H_{16}
9	Non	Nonene	Nonylene	C_9H_{18}
10	Dec	Decene	Decylene	$C_{10}H_{20}$

Figure 2.1: Alkene compounds

OLEFINIC HYDROCARBONS (ALKENES)

IUPAC Nomenclature

- A systematic method of naming organic chemical compounds as recommended by the International Union of Pure and Applied Chemistry also known as IUPAC.

- IUPAC which is a globally recognize international chemistry standards organizationthat has named all the chemical organic substances in a systematic manner.

- This particular naming standard for chemical organic substances is known as IUPAC nomenclature.

- IUPAC nomenclature is published in the Nomenclature of Organic Chemistry (also called the Blue Book).

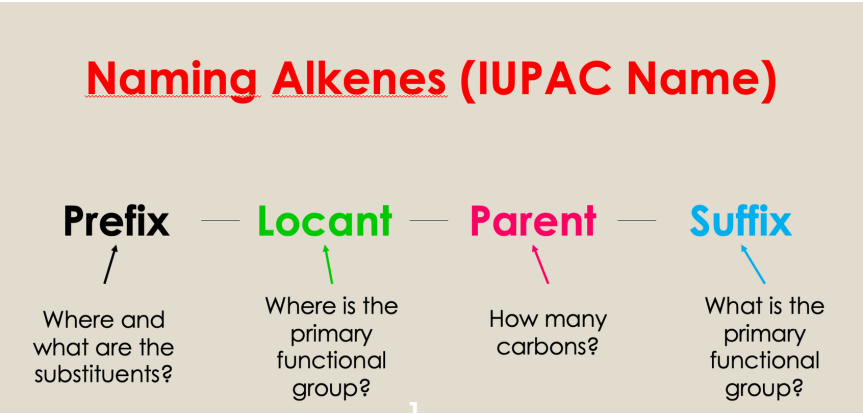


Figure 2.2: Four simple steps in naming Alkenes

OLEFINIC HYDROCARBONS (ALKENES)

Example 2.1

IUPAC Nomenclature

- Based on molecular structure below, it shows an alkene with a straight chain and the **number of carbon is 7**.

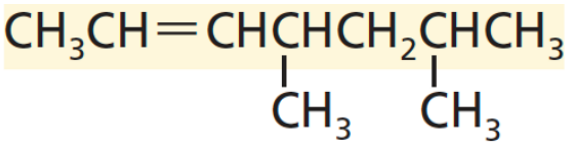
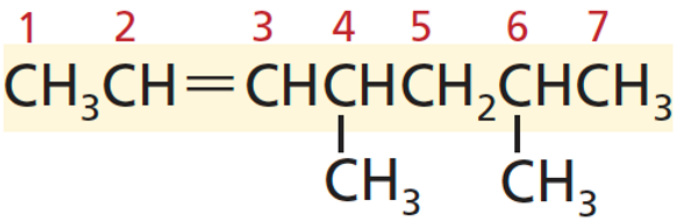


Figure 2.3: An alkene with 2 substituent and 1 double bond

- Herewith, given steps by steps to determine the IUPAC name for the molecular structure in **Figure 2.3**:

Step 1: Find the **parent** chain (longest chain of carbon).
Tips: 7 carbon of **longest straight chain**.
Answer: **Heptene**

Step 2: Determine the position of the **double bond**.
Tips: Number the chain to give the **lowest number** to the double bond.
Answer: **2**



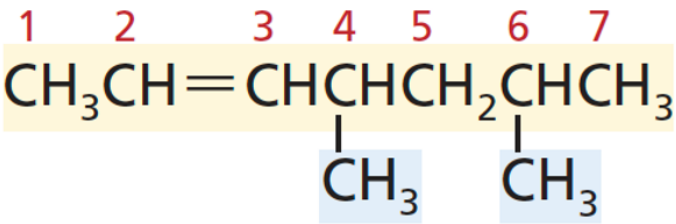
OLEFINIC HYDROCARBONS (ALKENES)

IUPAC Nomenclature

Step 3: **Name the alkene** based on double bond position.
Tips: Refer to answer in **step 1 and step 2**.
Answer: **Hept-2-ene**

Step 4: **Name** each **substituent and locate** its position.
Tips: Substituent **-CH3** is methyl and have **2 methyl**.
Tips: Substituent: **methyl**, Location: **4 and 6**
Numeric prefix: **di (two methyl)**
Answer: **4,6**
dimethyl
hept-2-ene

With that FOUR (4) Steps, the name of the alkene in **Figure 2.3** is **4,6-dimethyl-hept-2-ene**



OLEFINIC HYDROCARBONS (ALKENES)

Example 2.2

IUPAC Nomenclature

- Based on molecular structure below, it shows an alkene with a straight chain and the **number of carbon is 4**.

Figure 2.4: An alkene with 2 double bond

- Herewith, given steps by steps to determine the IUPAC name for the molecular structure in **Figure 2.4**:

Step 1: Find the **parent** chain (longest chain of carbon).
Tips: 4 carbon of **longest straight chain**.
Answer: **Butene**

Step 2: Determine the position of the **double bond**.
Tips: Number the chain to give the **lowest number** to the double bond.
Answer: **1 and 3 (1,3-di-ene)**

OLEFINIC HYDROCARBONS (ALKENES)

IUPAC Nomenclature

Step 3: **Name the alkene** based on double bond position.
Tips: Refer to answer in **step 1 and step 2**.
Answer: **Butene** and **1,3-di-ene**

Step 4: **Name** each **substituent and locate** its position.
Tips: **Add -a after but** (for double bond more than 1)
Answer: **Buta**
1,3
diene

With that FOUR (4) Steps, the name of the alkene in **Figure 2.4** is **buta-1,3-diene**

$$CH_2 = CHCH = CH_2$$

OLEFINIC HYDROCARBONS (ALKENES)

Example 2.3

IUPAC Nomenclature

- Based on molecular structure below, it shows an alkene with a straight chain and the **number of carbon is 7**.

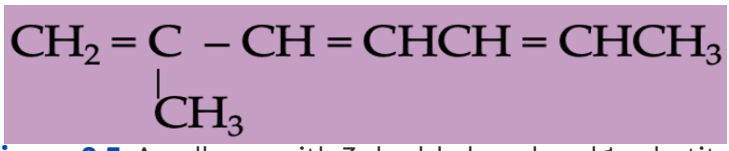
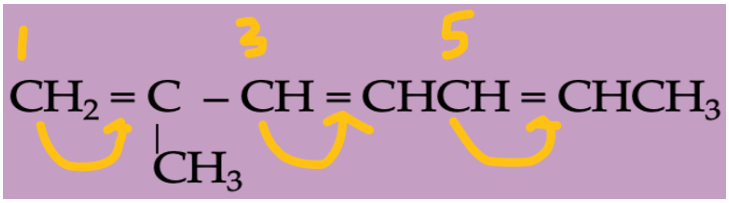


Figure 2.5: An alkene with 3 double bond and 1 substituent

- Herewith, given steps by steps to determine the IUPAC name for the molecular structure in **Figure 2.5**:

Step 1: Find the **parent** chain (longest chain of carbon).
Tips: 7 carbon of **longest straight chain**.
Answer: **Heptene**

Step 2: Determine the position of the **double bond**.
Tips: Number the chain to give the **lowest number** to the double bond.
Answer: **1,3,5 (1,3,5-tri-ene)**



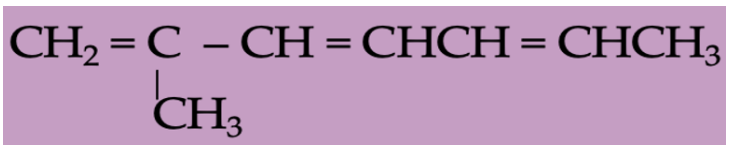
OLEFINIC HYDROCARBONS (ALKENES)

IUPAC Nomenclature

Step 3: **Name the alkene** based on double bond position.
Tips: Refer to answer in **step 1 and step 2**.
Answer: **Heptene** and **1,3,5-tri-ene**

Step 4: **Name** each **substituent and locate** its position.
Tips: **Add -a after hept** (for double bond more than 1)
Tips: Substituent: **methyl**, Location: **2**
Numeric prefix: **- (1 methyl)**
Answer: **1,3,5-tri-ene**
2-methyl
hepta

With that FOUR (4) Steps, the name of the alkene in **Figure 2.5** is **2-methyl-hepta-1,3,5-triene**



CYCLOALKENES

- Cycloalkenes are hydrocarbons containing a ring of carbon atoms and one or more double bonds in the cycle that do not form an aromatic ring.

- Cyclic unsaturated hydrocarbon having general molecular formula CnH2n-2.

- Cycloalkenes are named by the system used for the open-chain alkenes, except that numbering always is started at one of the carbons of the double bond and continued around the ring through the double bond so as to keep the index numbers as small as possible.

- Many compounds contain two or more double bonds and are known as alkadienes, alkatrienes, alkatetraenes, and so on, the suffix denoting the number of double bonds.

CYCLOALKENES

Example 2.4

IUPAC Nomenclature

- Based on molecular structure below, it shows a cycloalkene with a substituent of a functional group.

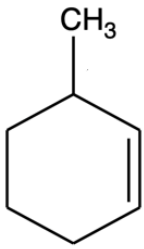


Figure 2.6: A cycloalkene with 1 double bond and 1 substituent

- Herewith, given steps by steps to determine the IUPAC name for the molecular structure in **Figure 2.6**:

Step 1: Find the **parent** chain (longest chain of carbon).
Tips: **Number** the carbon atoms in the ring so that **double bond is between carbon atom 1 and 2.**
Answer: **Cyclohexene**

Step 2: Give **lower numbers to the functional group**.
Tips: **Nearest** double bond to the methyl group.
Answer: **3-methyl**

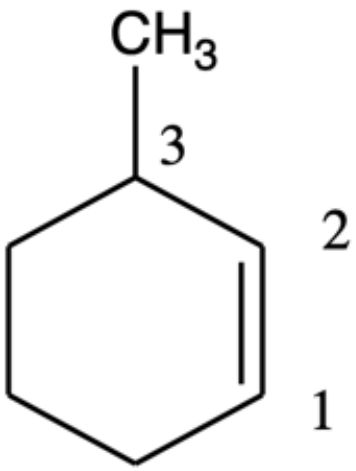
CYCLOALKENES

IUPAC Nomenclature

Step 3: **Name the cycloalkene** based on double bond.
Tips: Refer to answer in **step 1 and step 2**.
Answer: **Cyclohexene** and **3-methyl**

Step 4: **Number and list groups in alphabetical order**.
Tips: Substituent: **methyl**, Location: **3**
Numeric prefix: **- (1 methyl)**
Answer: **3-methyl**
Cyclohex-1-ene

With that FOUR (4) Steps, the name of the cycloalkene in **Figure 2.6** is **3-methylcyclohex-1-ene**



CYCLOALKENES

Example 2.5

IUPAC Nomenclature

- Based on molecular structure below, it shows a cycloalkene with a substituent of a functional group.

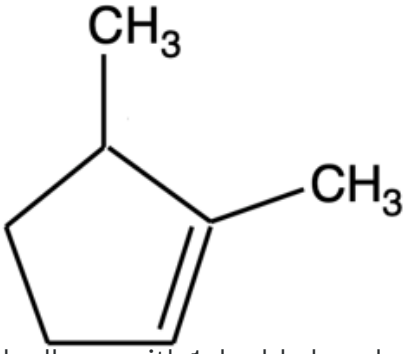


Figure 2.7: A cycloalkene with 1 double bond and 2 substituent

- Herewith, given steps by steps to determine the IUPAC name for the molecular structure in **Figure 2.7**:

Step 1: Find the **parent** chain (longest chain of carbon).
Tips: **Number** the carbon atoms in the ring so that **double bond is between carbon atom 1 and 2.**
Answer: **Cyclohexene**

Step 2: Give **lower numbers to the functional group**.
Tips: **Nearest** double bond to the methyl group.
Answer: **1,5-dimethyl**

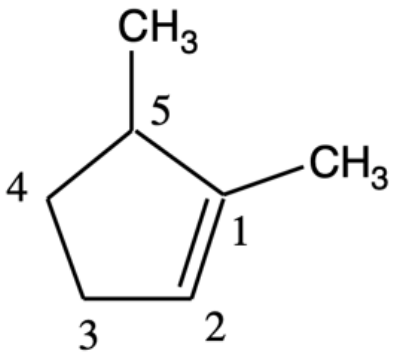
CYCLOALKENES

IUPAC Nomenclature

Step 3: **Name the cycloalkene** based on double bond.
Tips: Refer to answer in **step 1 and step 2**.
Answer: **Cyclohexene** and **1,5-dimethyl**

Step 4: **Number and list groups in alphabetical order**.
Tips: Substituent: **methyl**, Location: **1 and 5**
Numeric prefix: **di (2 methyl)**
Answer: **1,5-dimethyl**
Cyclohex-1-ene

With that FOUR (4) Steps, the name of the cycloalkene in **Figure 2.7** is **1,5-dimethylcyclohex-1-ene**



CYCLOALKENES

Example 2.6

IUPAC Nomenclature

- Based on molecular structure below, it shows a cycloalkene with a substituent of a functional group.

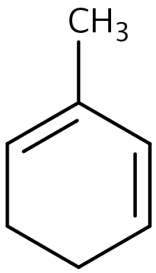


Figure 2.8: A cycloalkene with 2 double bond and 1 substituent

- Herewith, given steps by steps to determine the IUPAC name for the molecular structure in **Figure 2.8**:

Step 1: Find the **parent** chain (longest chain of carbon).
Tips: **Number** the carbon atoms in the ring so that **double bond is between carbon atom 1 and 2.**
Answer: **Cyclohexene**

Step 2: Give **lower numbers to the functional group**.
Tips: **Nearest** double bond to the methyl group (location: 2).
Answer: **2-methyl**

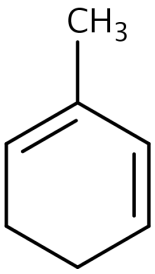
CYCLOALKENES

IUPAC Nomenclature

Step 3: **Name the cycloalkene** based on double bond.
Tips: Refer to answer in **step 1 and step 2**.
Tips: 2 double bond (location: **1 and 3**).
Answer: **Cyclohexene, 1,3-diene** and **2-methyl**

Step 4: **Number and list groups in alphabetical order**.
Tips: Substituent: **methyl**, Location: **2**
Numeric prefix: **- (1 methyl)**
Tips: Add -a after cyclohex (double bond more than 1).
Answer: **2-methyl**
Cyclohexa
1,3-diene

With that FOUR (4) Steps, the name of the cycloalkene in **Figure 2.8** is **2-methylcyclohexa-1,3-diene**



Physical Properties of Alkenes

- Insoluble in water but soluble in organic solvent.
- Low densities (less dense than water).
- Low melting point and boiling point. The boiling point and melting point of an alkene is usually lower than alkane with same number of atom.

IUPAC Name	Molecular Formula	Condensed Structural Formula	Melting Point (°C)	Boiling Point (°C)
Ethene	C_2H_4	$CH_2=CH_2$	-169	-104
Propene	C_3H_6	$CH_2=CHCH_3$	-185	-47
1-butene	C_4H_8	$CH_2=CHCH_2CH_3$	-185	-6
1-pentene	C_5H_{10}	$CH_2=CH(CH_2)_2CH_3$	-138	30
1-hexene	C_6H_{12}	$CH_2=CH(CH_2)_3CH_3$	-140	63
1-heptene	C_7H_{14}	$CH_2=CH(CH_2)_4CH_3$	-119	94
1-octene	C_8H_{16}	$CH_2=CH(CH_2)_5CH_3$	-102	121

Figure 2.9: Physical properties of alkenes

- Inflammable.
- At room temperature:
  C2-C4 Gas
  C5-C16 Liquids

Physical Properties of Cycloalkenes

- Cycloalkenes are unsaturated and therefore have fewer hydrogen atoms and fewer bonds, as opposed to open-chain alkenes, which means that there is less internal energy within the molecule.
- Like cycloalkanes, cycloalkenes use Van der Waals forces to bond.
- Macroscopically, most cycloalkenes are liquid at room temperature, though have very low solubility in water.
- Only the first few cycloalkenes are gases.
- Cycloalkenes are rarely solid at room temperature.
- Essentially, cycloalkenes have similar physical properties to alkenes and cycloalkanes aside from the fact that cycloalkenes have at least one double bond.

Chemical Properties of Alkenes

- Alkenes are unsaturated compound, which makes them highly reactive than alkanes.

- Alkenes can undergo four major type of reactions:
  a) Combustion reactions.
  b) Addition reactions
    i. Halogenation
    ii. Hydration
    iii. Hydrohalogenation
    iv. Hydrogenation

Type of reaction	Reactant	Main product	By-product	Chemical Reaction
Combustion				
Combustion (complete)	Oxygen, O_2	Carbon dioxide, CO_2	Water, H_2O	$C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2\ H_2O$
Combustion (incomplete)	Oxygen, O_2	Carbon monoxide, CO	Water, H_2O	$C_2H_4 + 2O_2 \rightarrow 2CO + 2H_2O$
		Carbon, C	Water, H_2O	$C_2H_4 + O_2 \rightarrow 2C + 2H_2O$
Addition				
Halogenation	Bromine gas, Br_2	1,1-dibromoethane, $C_2H_4Br_2$	-	$C_2H_4 + Br_2 \rightarrow C_2H_4Br_2$
	Chlorine gas, Cl_2	1,1-dichloroethane, $C_2H_4Cl_2$	-	$C_2H_4 + Cl_2 \rightarrow C_2H_4Cl_2$
	Iodine gas, I_2	1,1-diiodooethane, $C_2H_4I_2$	-	$C_2H_4 + I_2 \rightarrow C_2H_4I_2$
Hydration	Water, H_2O	Alcohol (Ethanol), $C_nH_{2n+1}OH$ C_2H_5OH	-	$C_2H_4 + H_2O \rightarrow C_2H_5OH$
Hydrohalogenation	Hydrogen bromide, HBr	Bromoethane, C_2H_5Br	-	$C_2H_4 + HBr \rightarrow C_2H_5Br$
	Hydrogen chloride, HCl	Chloroethane, C_2H_5Cl	-	$C_2H_4 + HCl \rightarrow C_2H_5Cl$
Hydrogenation	Hydrogen gas (H_2)	Alkane C_nH_{2n+2}	-	$C_2H_4 + H_2 \rightarrow C_2H_6$

Figure 2.10: Chemical properties of ethene

Chemical Properties of Cycloalkenes

- The smaller the ring, the more likely it is to undergo reactions due to the carbon carbon bond angle.
- Cyclopropene is very reactive and has an extremely high strain. Larger compounds show very little ring strain and are less reactive.
- Undergo combustion and halogenation reactions.
- Cycloalkenes generally are more reactive than cycloalkanes due to their double carbon-carbon bond.
- It also undergo addition reactions, which occurs when the pi bond is broken and two new sigma bonds are formed.

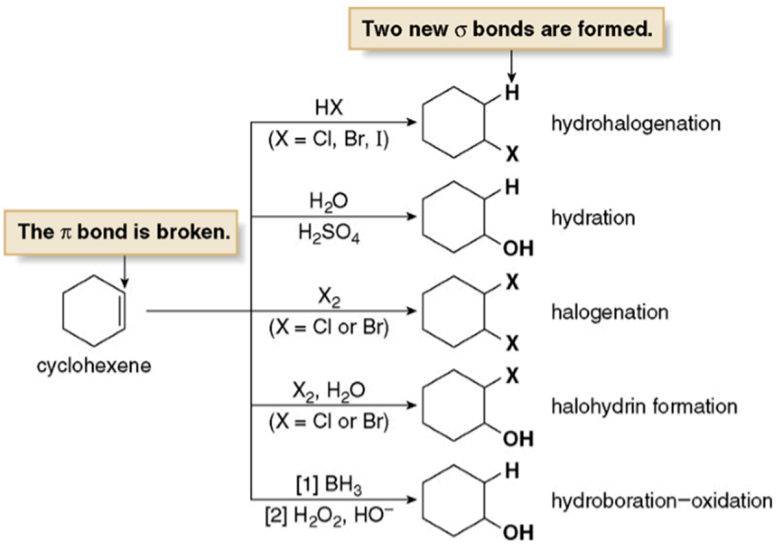


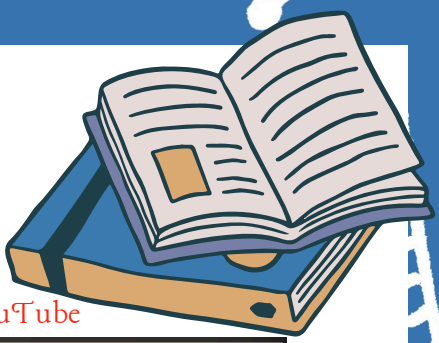
Figure 2.11: Chemical properties of cyclohexene

CHEMISTRY OF PETROCHEMICAL PROCESSES, VOL. 1

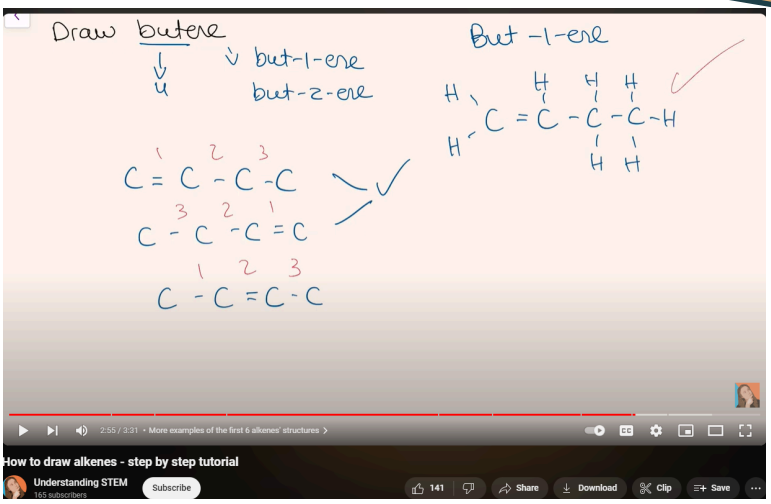
Chapter 4

Olefinic Hydrocarbons

Interactive Activities 2



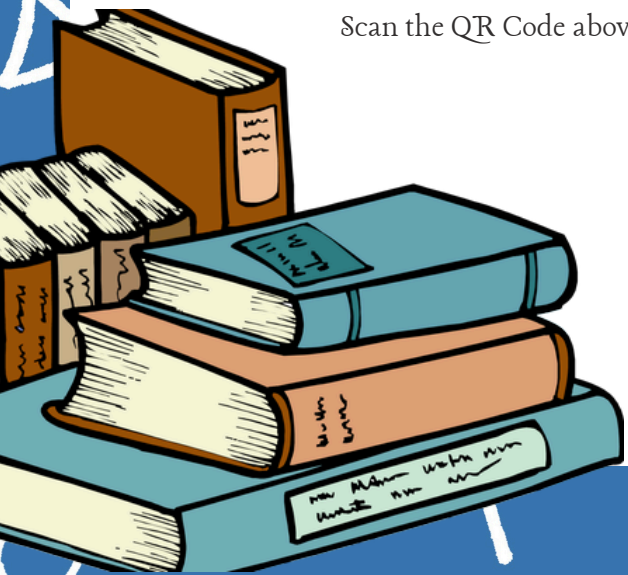
Watch Alkene Tutorial on YouTube



Scan the QR Code above for the alkene interactive video

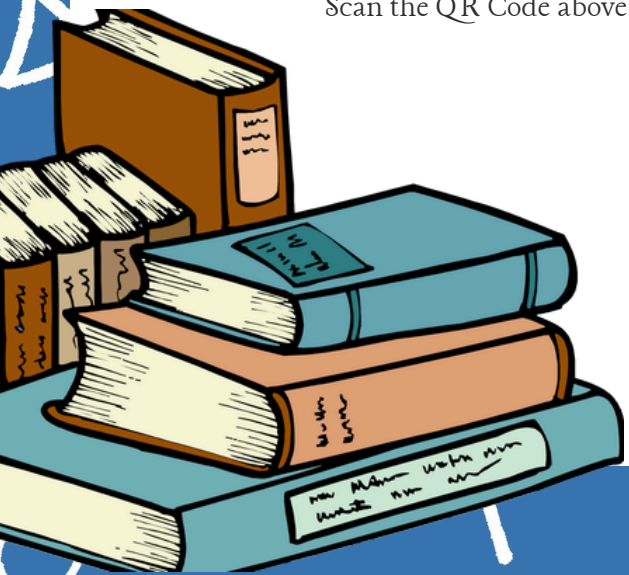
Class Activity: Intro and Properties of Alkene

Scan the QR Code above to answer the Quiz



Class Activity: IUPAC name of Alkenes

Scan the QR Code above to answer the Quiz



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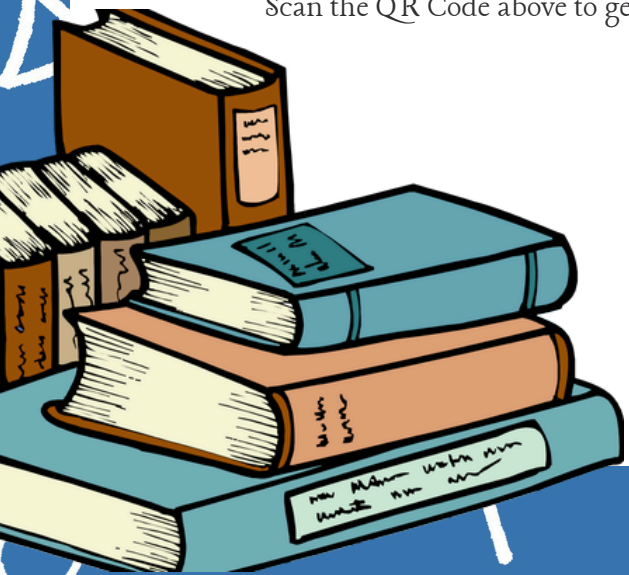

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