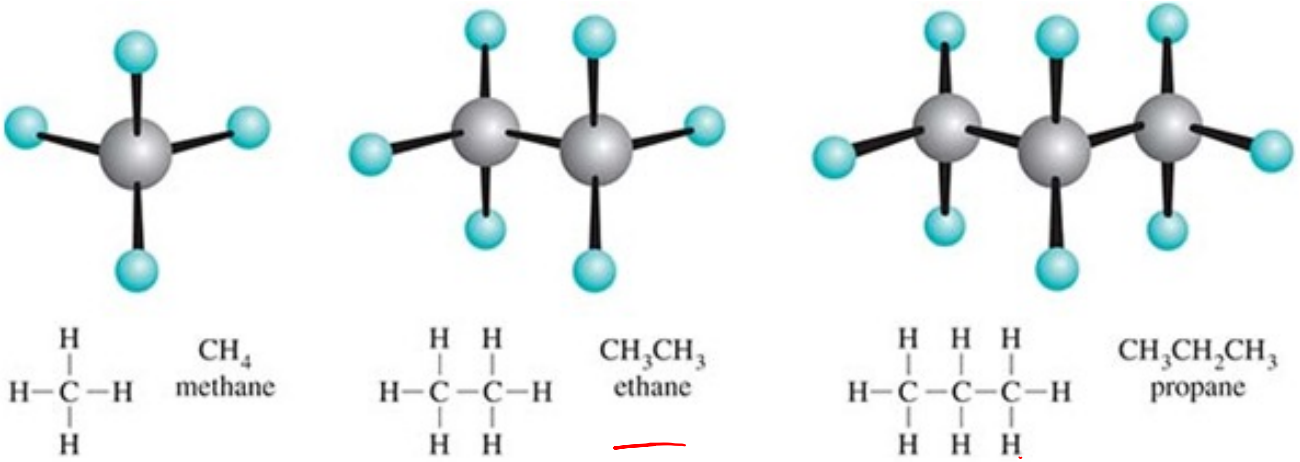
Saturated Hydrocarbons

Alkanes



Hein * Pattison * Arena * Best *

19.5 Hydrocarbons

19.6 Saturated Hydrocarbons: Alkanes
19.7 Carbon Bonding in Alkanes Isomerism
19.9 Naming Organic Compounds
19.11 Reactions of Alkanes
19.12 Sources of Alkanes
19.13 Gasoline: A Major Petroleum Product
19.14 Cycloalkanes

Introduction to the Reactions of Carbon

19.11 Reactions of Alkanes
19.12 Sources of Alkanes
19.13 Gasoline: A Major Petroleum Product
19.14 Cycloalkanes

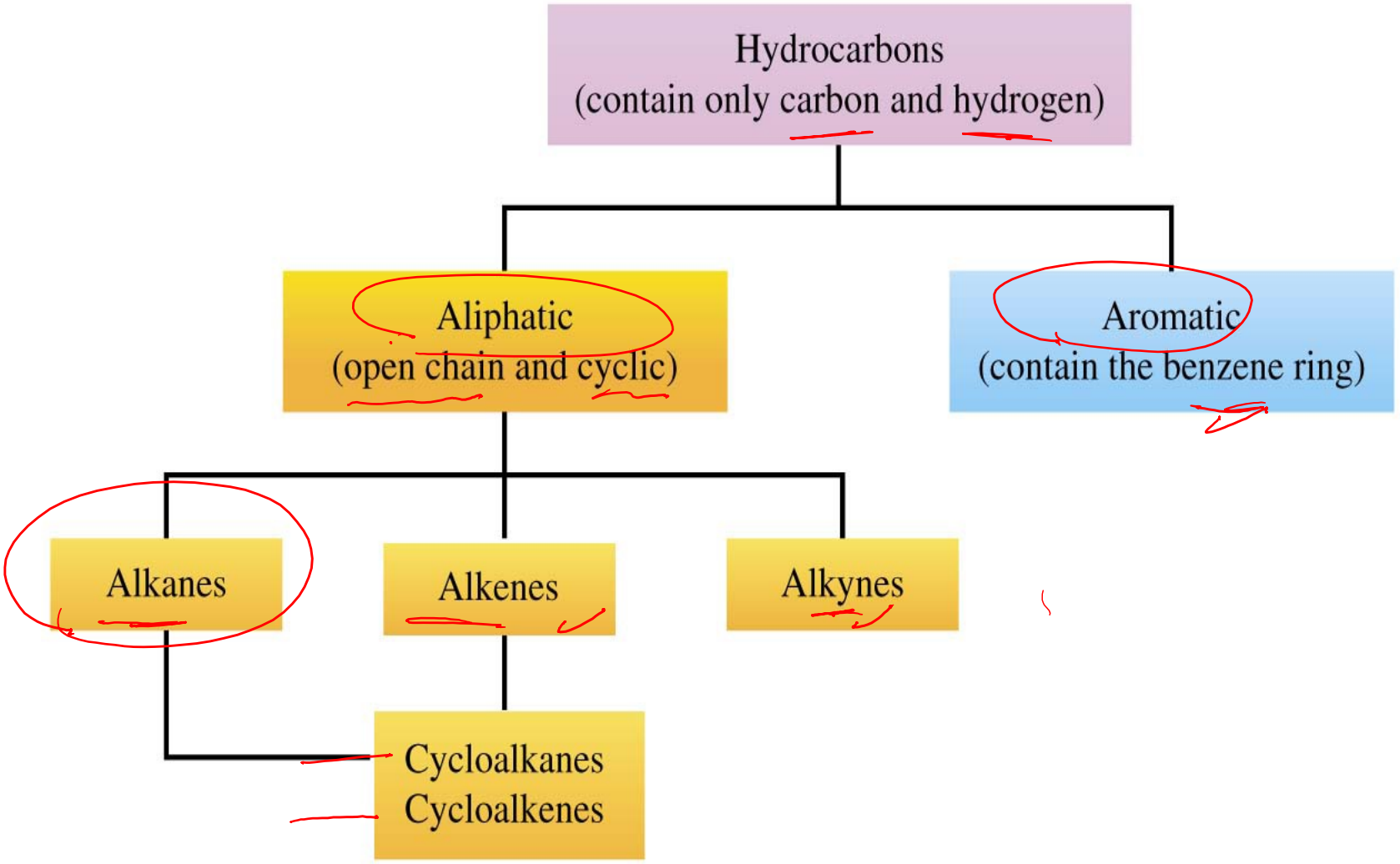
Hydrocarbons

Hydrocarbons are organic compounds that contain only carbon and hydrogen atoms. *(e.g. propane-$CH_3CH_2CH_3$ is a hydrocarbon but ethanol CH_3CH_2OH is not)*

Hydrocarbons are classified as either aliphatic *(i.e those hydrocarbons without benzene rings in the chemical structure)* or aromatic.*(i.e those hydrocarbons with benzene rings in the chemical structure)* as shown in Figure 19.5 in the next slide.

Hydrocarbons are also classified as saturated or unsaturated compounds

Figure 19.4 Classes of Hydrocarbons



Hydrocarbons

The principal source of hydrocarbons is fossil fuels which include natural gas, petroleum, and coal.

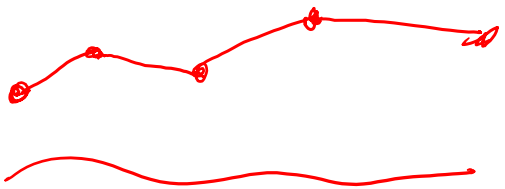
Fossil fuels are the primary source of heat and also a primary source of organic chemicals.

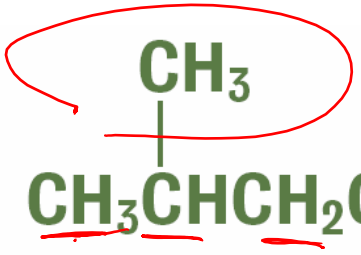
19.6 Saturated Hydrocarbons: Alkanes

Alkanes are saturated hydrocarbons that are either straight- chain or branched-chain hydrocarbons.

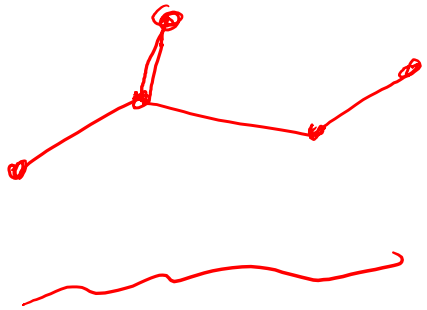
$CH_3CH_2CH_2CH_2CH_3$

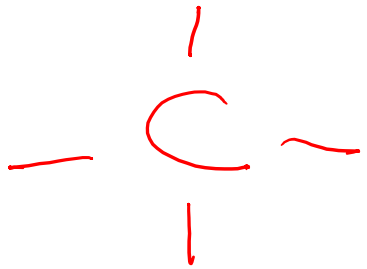
straight–carbon chain

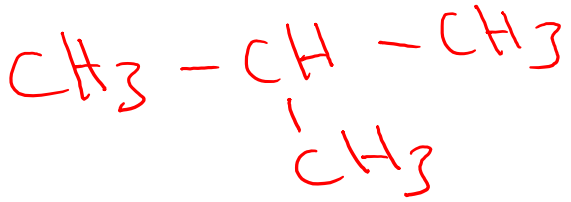


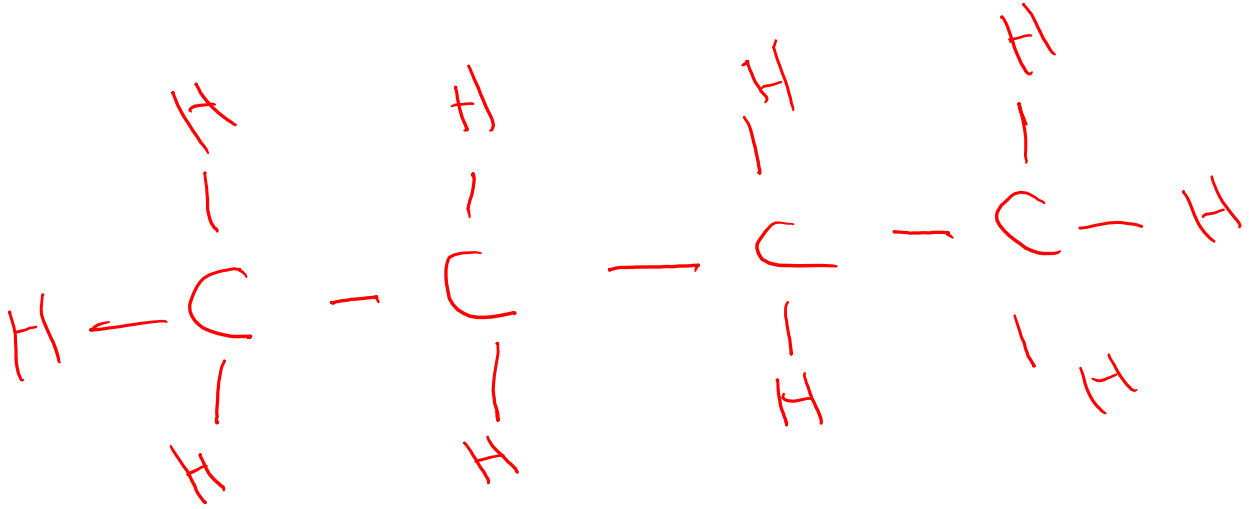


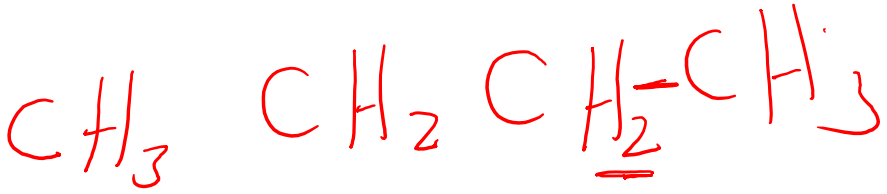
branched–chain of carbon atoms

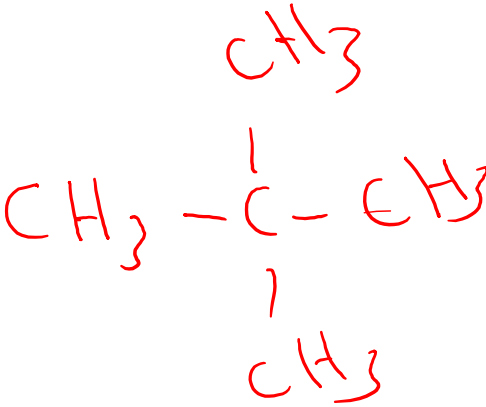












Homologous Series

Alkanes form a homologous series as seen in Table 19.2. Members of a homologous series have similar structures but different chemical formulas.

The general formula for the homologous series of open-chain alkanes is shown here.

$$C_nH_{2n+2}$$

general formula for open-chain alkanes

C_nH_{2n+2} Alkane

→ CH_4

→ C_2H_6 CH_3-CH_3

→ C_3H_8 $CH_3CH_2CH_3$

→ C_4H_{10} $CH_3CH_2CH_2CH_3$

→ C_5H_{12}

→ C_6H_{14}

$CH_3CH_2CH_2CH_2CH_2CH_3$

Table 19.2 Names, Formulas of Straight-Chain Alkanes

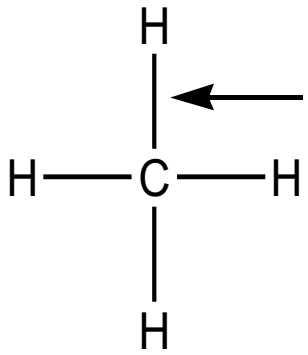
Name	Molecular formula C_nH_{2n+2}	Condensed structural formula
Methane	CH_4	CH_4
Ethane	C_2H_6	CH_3CH_3
Propane	C_3H_8	$CH_3CH_2CH_3$
Butane	C_4H_{10}	$CH_3CH_2CH_2CH_3$
Pentane	C_5H_{12}	$CH_3CH_2CH_2CH_2CH_3$
Hexane	C_6H_{14}	$CH_3CH_2CH_2CH_2CH_2CH_3$
Heptane	C_7H_{16}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_3$
Octane	C_8H_{18}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$
Nonane	C_9H_{20}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$
Decane	$C_{10}H_{22}$	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$

19.7 Carbon Bonding in Alkanes

Alkanes contain saturated carbon atoms that have four sigma bonds

Sigma bonds are linear bonds formed by a pair of electrons in overlapping atomic orbitals.

Carbon has the ability to form two, three, or four sigma bonds because of its ability to hybridize its valence shell electron orbitals



Each C-H sigma bond is formed by overlap of H_{1s} and C_{sp3} orbitals

methane

(an alkane)

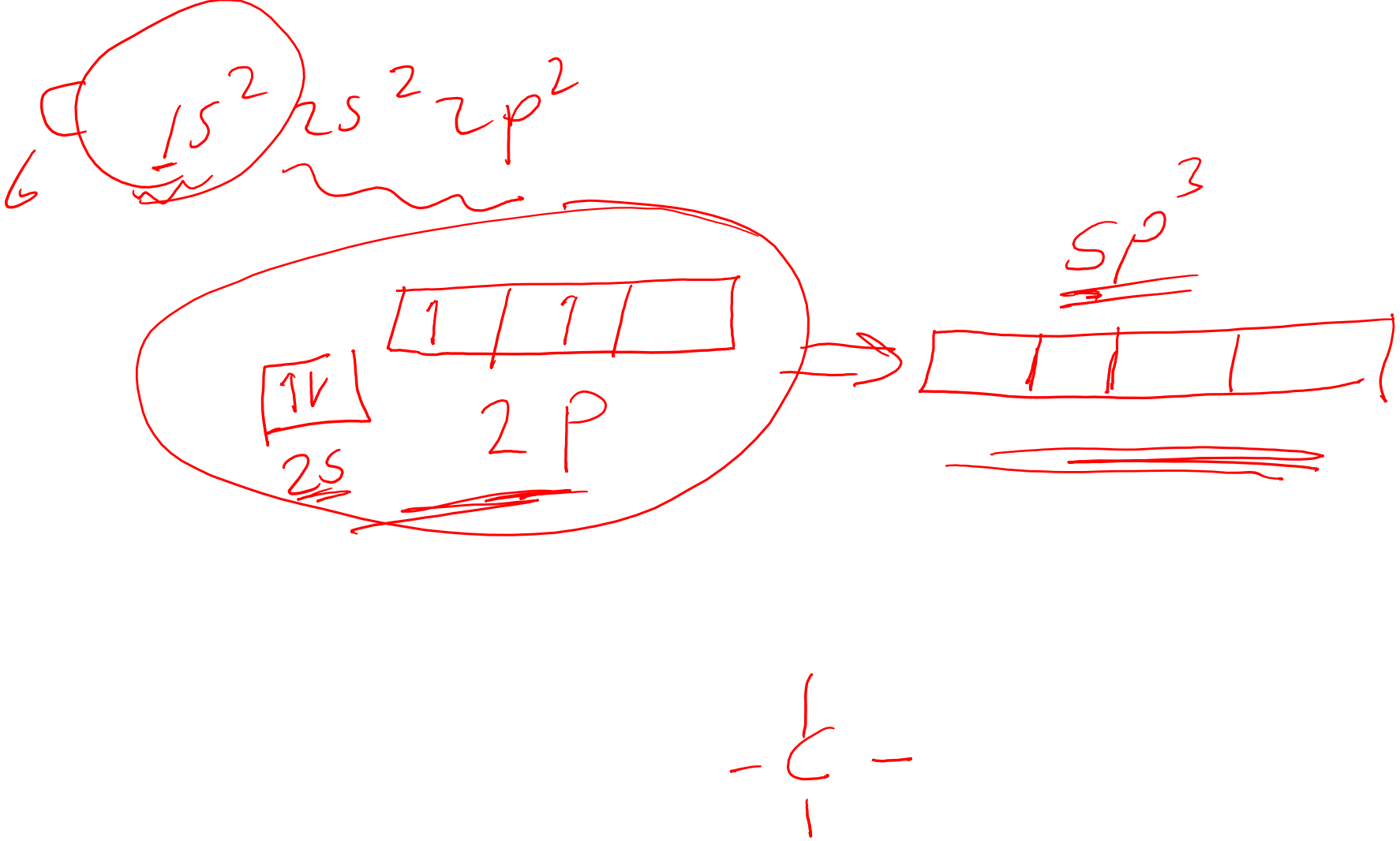
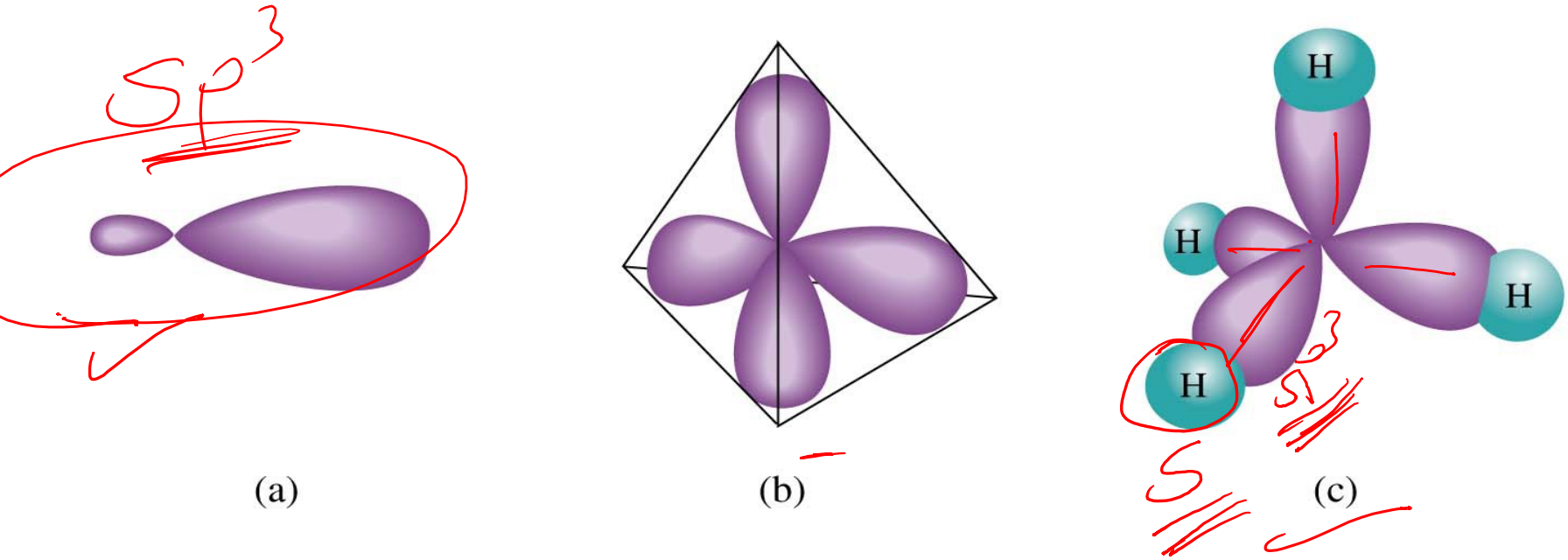
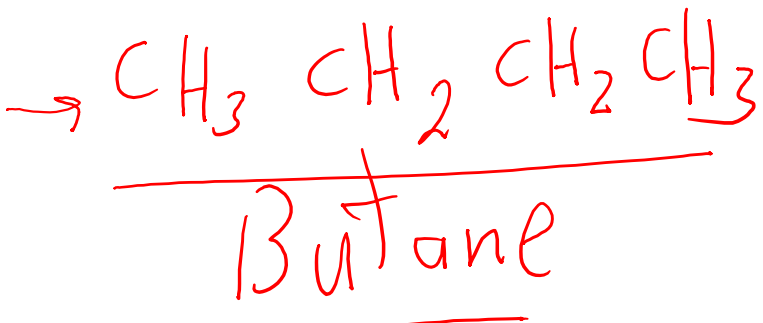
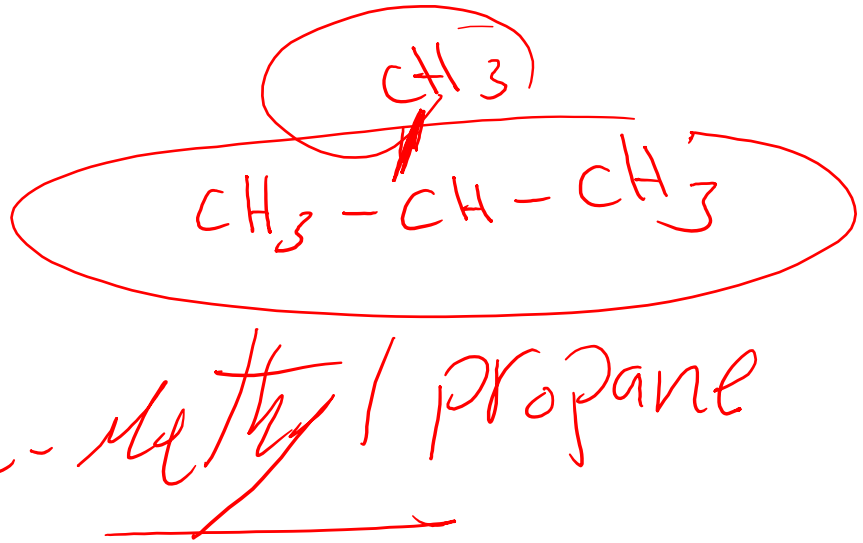

6
$1s^2 2s^2 2p^2$
2s
2p
sp^3

Figure 19.6 (a) A single sp^3-hybridized orbital; (b) four sp^3-hybridized orbitals in a tetrahedral arrangement; (c) sp^3 and s orbitals overlapping to form four C-H sigma bonds in methane.



(a) (b) (c)

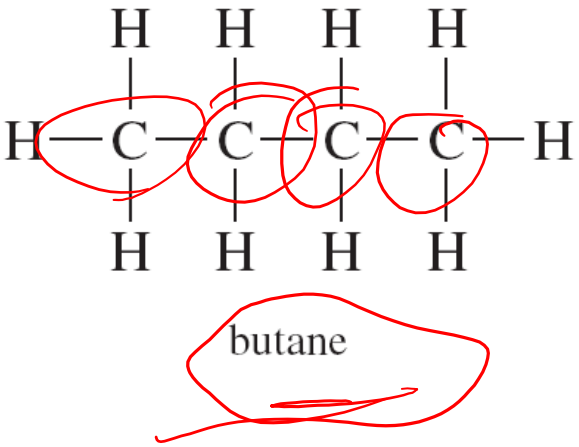




19.8 Isomerism

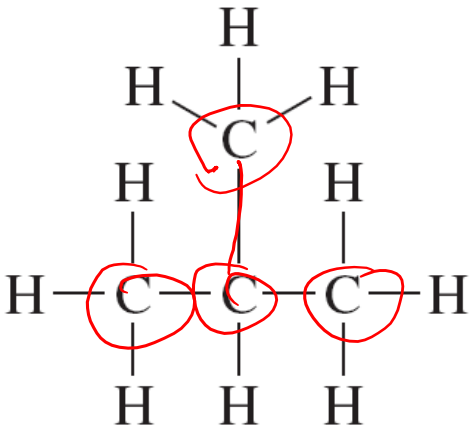
Open-chain alkanes with four or more carbon atoms can form isomers. Isomers are molecules that have the same number and same type of atoms but the atoms are connected differently.

For example, it is possible to write two structural formulas corresponding to the molecular formula C_4H_{10} i.e., butane and isobutane which are isomers of each other.



butane

and



isobutane

C_5H_8 ×

C_5H_{12} ✓

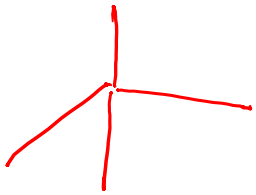
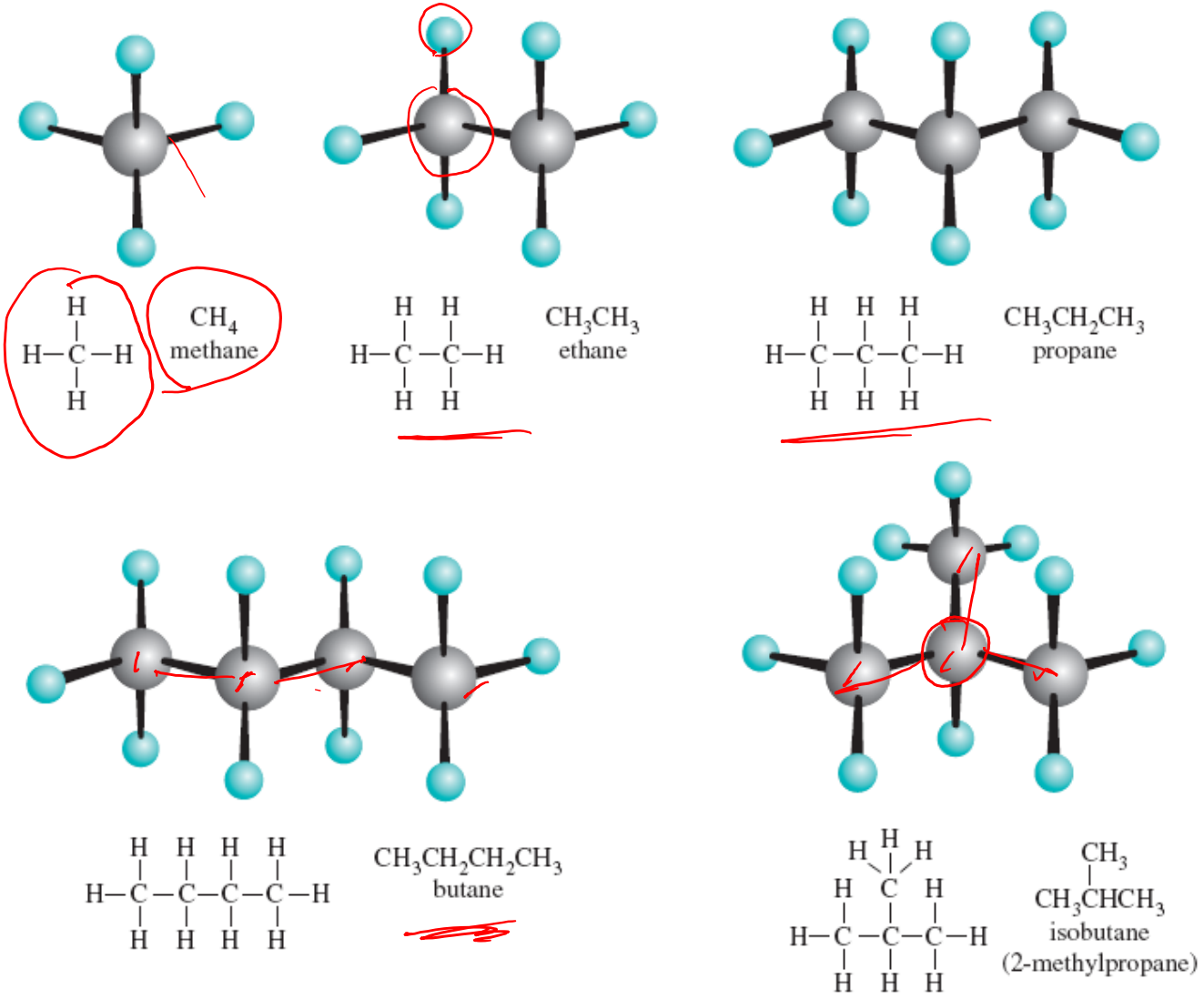
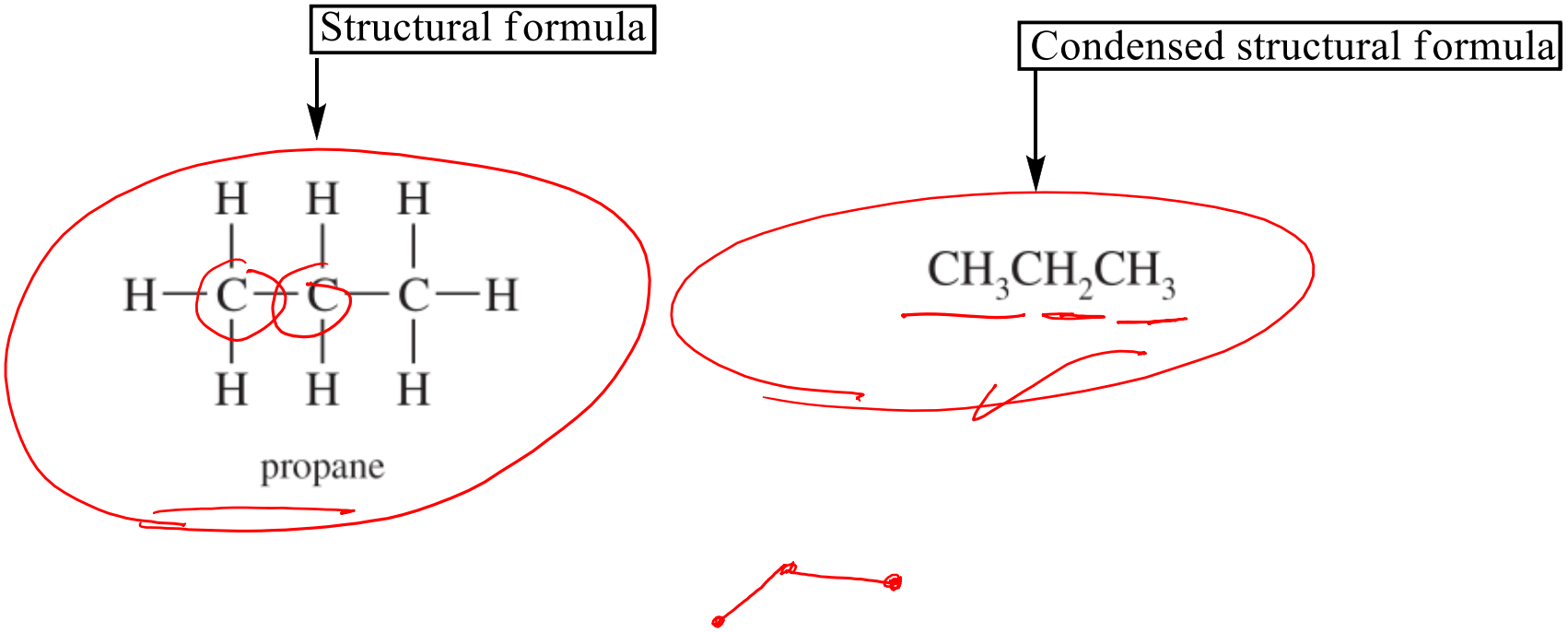


Figure 19.7 Ball-and-stick models illustrating the structural formulas of several alkanes.

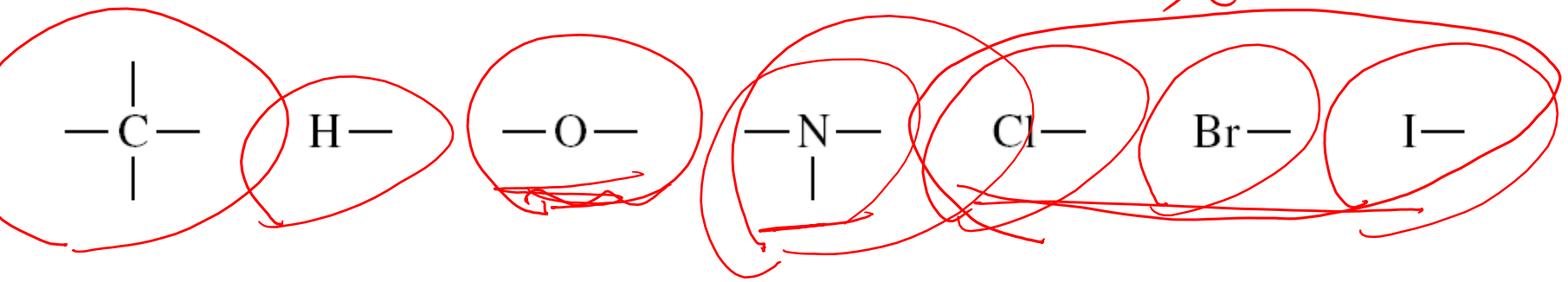


Organic chemists often write structural formulas as condensed structural formulas to save time.



Alkanes are nonpolar compounds with low boiling points.

Many organic compounds are derivatives of alkanes. Many of these compounds have one or more of the following elements in them.



The dashed lines indicate the number of bonds each element can form. For example nitrogen can form three bonds while oxygen can only form two bonds.

19.9 Naming Organic Compounds

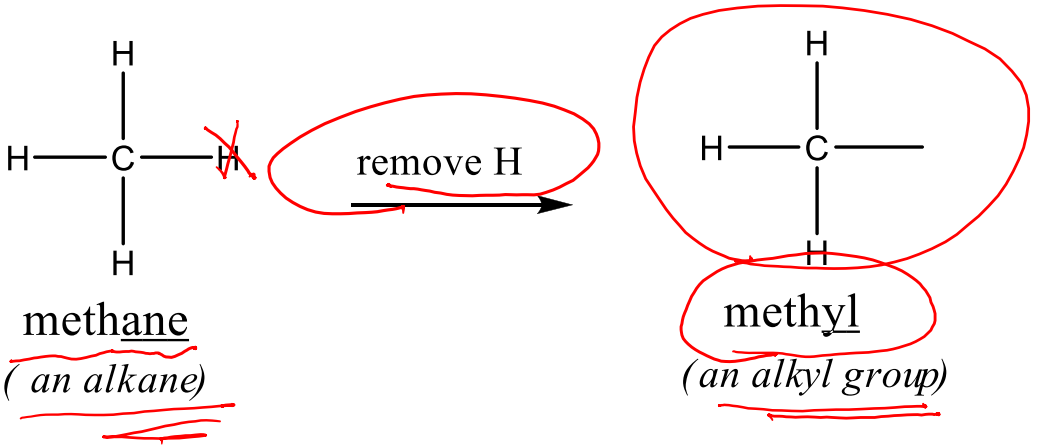
How do chemist name organic compounds ?

Organic compounds are named using the IUPAC System *(International Union of Pure and Applied Chemistry).*

The IUPAC System was developed at an international science meeting in Geneva in 1892 . The IUPAC System is essentially a set of rules that allow for a systematic and uniform method of naming compounds.

Naming Alkyl Groups

Alkyl groups have one hydrogen less than the respective alkane.



The general formula for alkyl groups is shown here and a list of alkyl groups are shown in Table 19.3 .

$$R = C_nH_{2n+1}$$

- CH_3-

- CH_3CH_2-

- $CH_3CH_2CH_2-$

Propyl

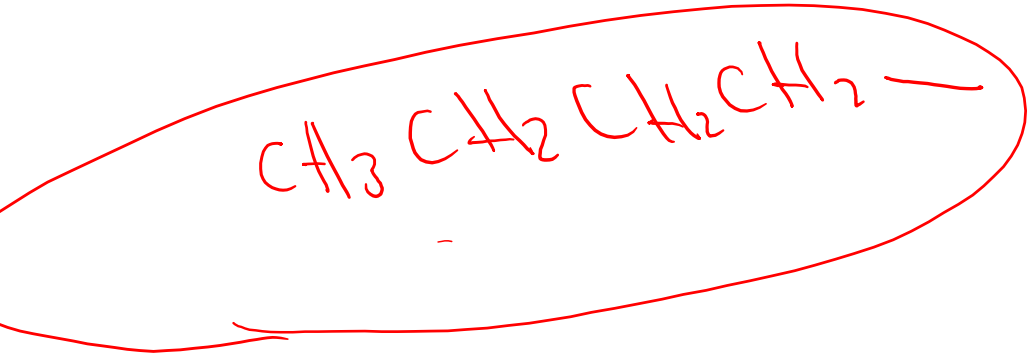
$CH_3-\underset{|}{CH}-CH_3$

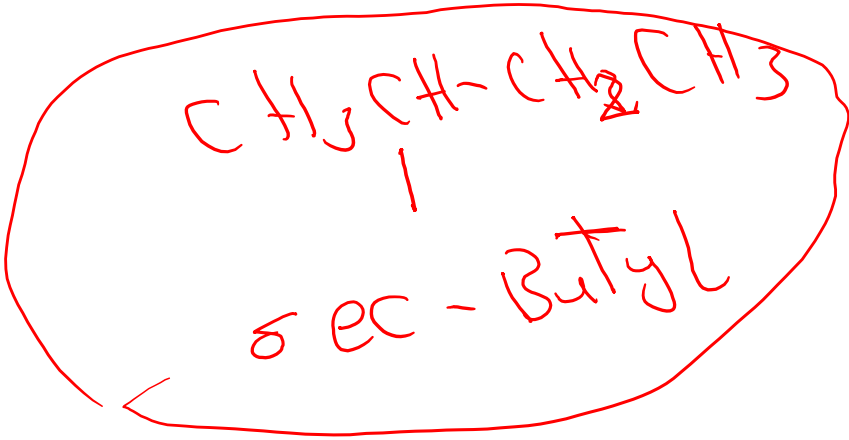
Isopropyl

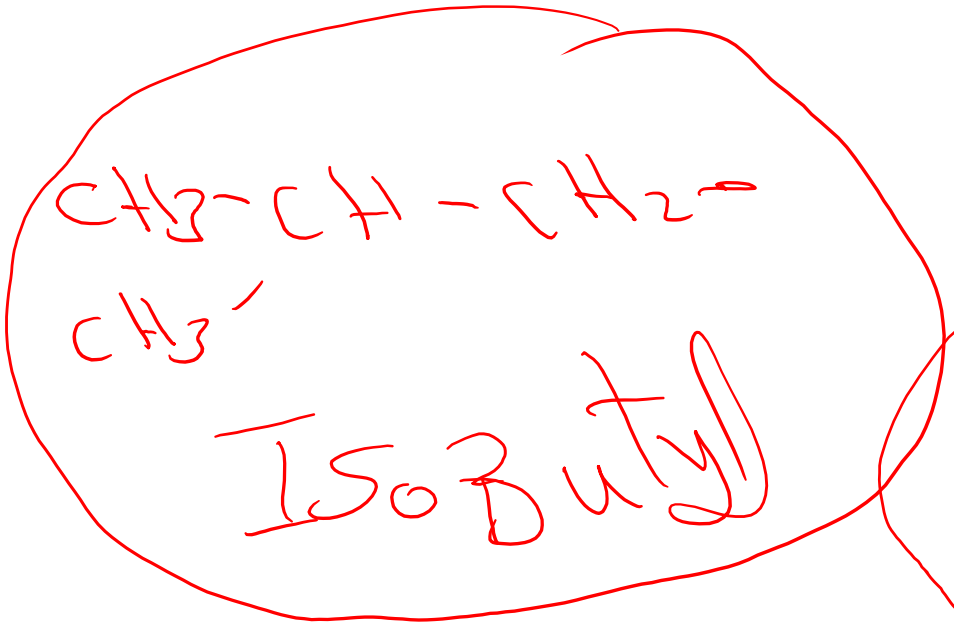
- $CH_3CH_2CH_2CH_2-$

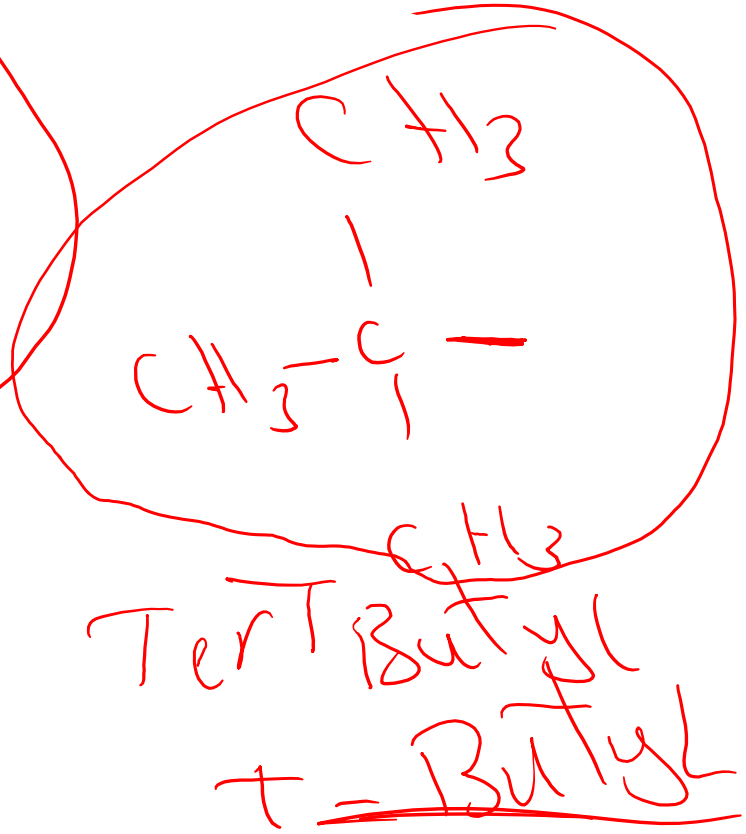
Table 19.3 Names and Formulas of Selected Alkyl Groups

Formula	Name	Formula	Name
CH_3-	methyl	$CH_3CH(CH_3)-$	isopropyl
CH_3CH_2-	ethyl	CH_3CHCH_2- (CH$_3$ branch)	isobutyl
$CH_3CH_2CH_2-$	propyl	$CH_3CH_2CH(CH_3)-$	*sec*-butyl (secondary butyl)
$CH_3CH_2CH_2CH_2-$	butyl	$CH_3C(CH_3)_2-$	*tert*-butyl or *t*-butyl (tertiary butyl)
$CH_3(CH_2)_3CH_2-$	pentyl		
$CH_3(CH_2)_4CH_2-$	hexyl		
$CH_3(CH_2)_5CH_2-$	heptyl		
$CH_3(CH_2)_6CH_2-$	octyl		
$CH_3(CH_2)_7CH_2-$	nonyl		
$CH_3(CH_2)_8CH_2-$	decyl		


CH3CH2CH2CH2—


CH3CH—CH2CH3
sec-Butyl

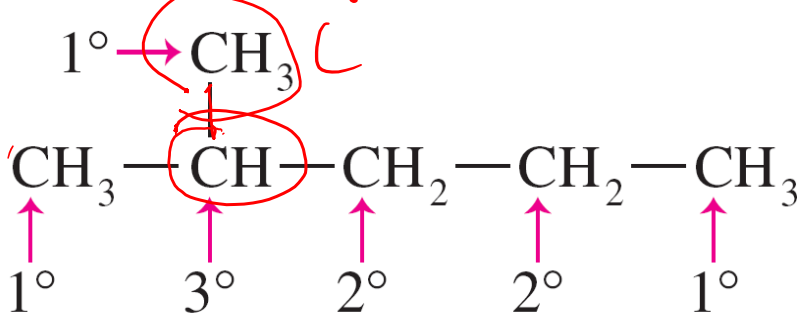

CH3—CH—CH2—
CH3
IsoButyl

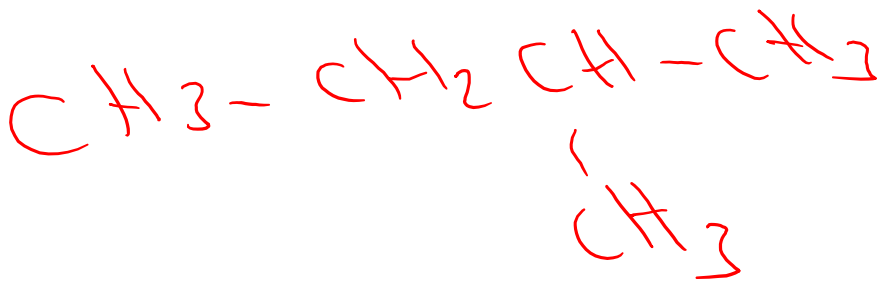

CH3
CH3—C—
CH3
TerTButyl
t-Butyl

Carbon atoms are often classified in this way:

Primary (1°)	A carbon with <u>one</u> carbon attached
Secondary (2°)	A carbon with <u>two</u> carbons attached
Tertiary (3°)	A carbon with <u>three</u> carbons attached

Here is an example of a molecule with all three types of carbons.





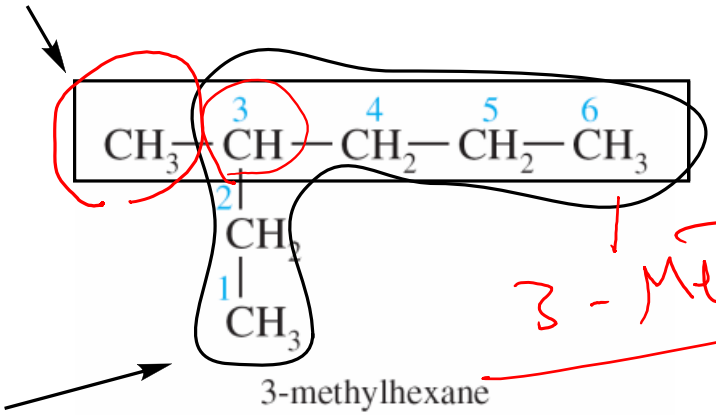
1° 2° 3°

@chem3_phys

IUPAC Rules for Naming Alkanes

1. Identify and then name the longest continuous chain.

This would not be the longest chain *(i.e. only five carbon atoms)*



3-methylhexane

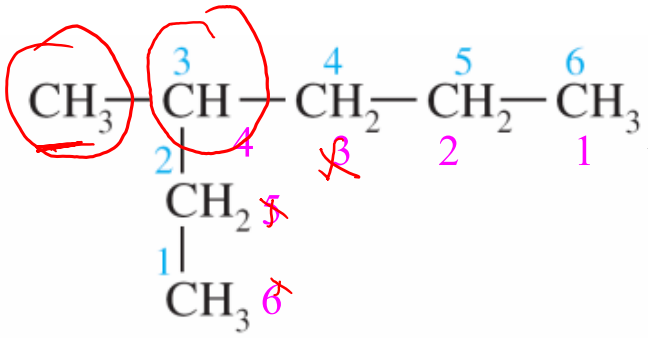
This is the longest chain

3-Methylhexane

$CH_3-CH_2-CH(CH_2CH_2CH_3)-CH_2-CH_3$

IUPAC Rules for Naming Alkanes

2. Number the chain so any branch alkyl groups have the lowest possible number.

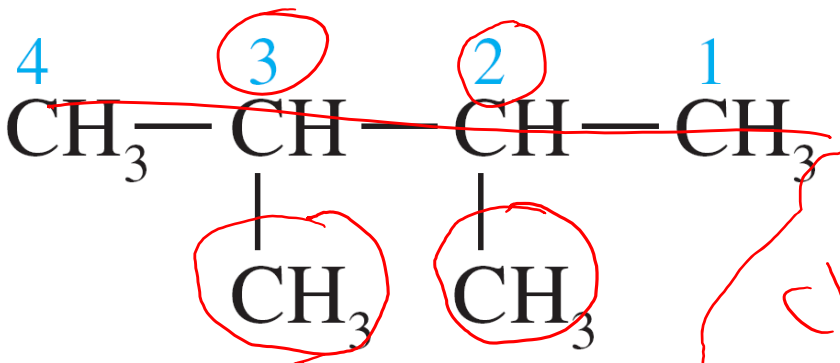


Numbering in this direction is incorrect because it gives the methyl branch a higher number, i.e. a 4 instead of a 3.

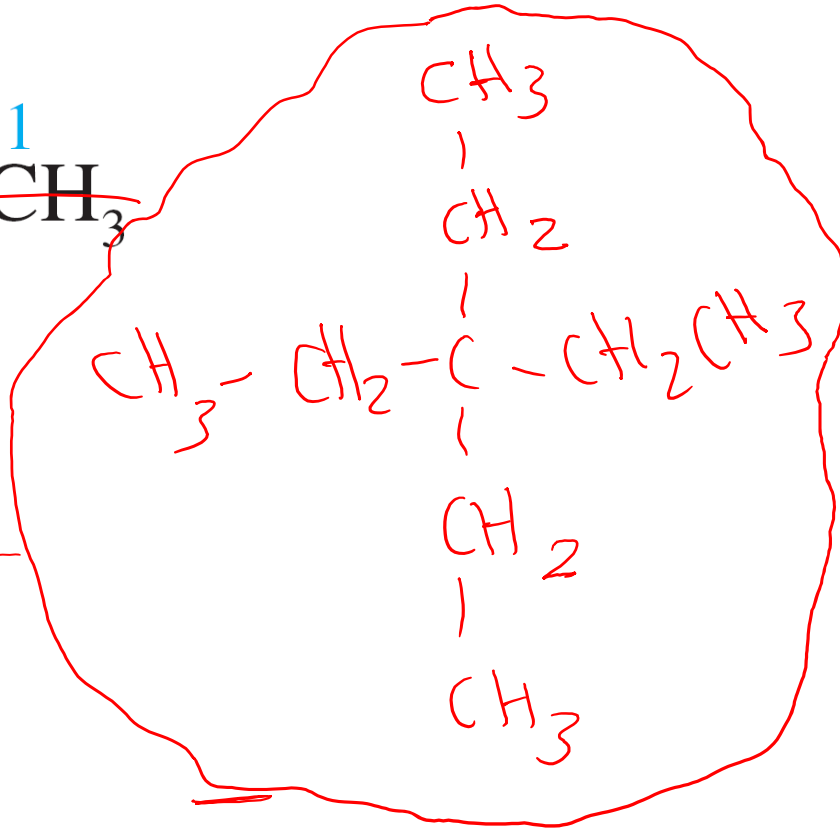
IUPAC Rules for Naming Alkenes

3. Use prefixes if two or more *(i.e. di, tri, tetra etc.)* of the same alkyl group branches appear on the chain.

2,3 - dimethyl butane

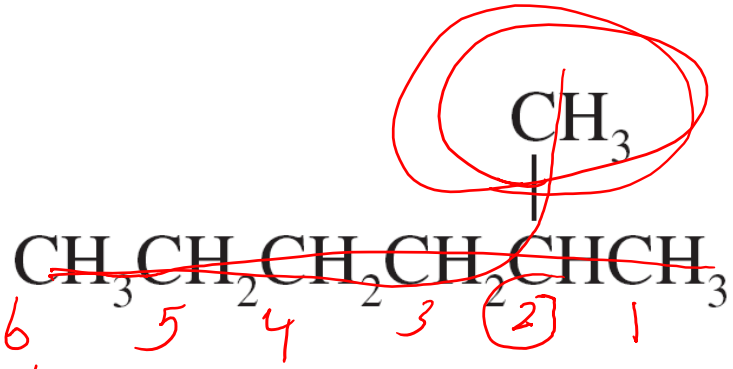


2,3-dimethylbutane



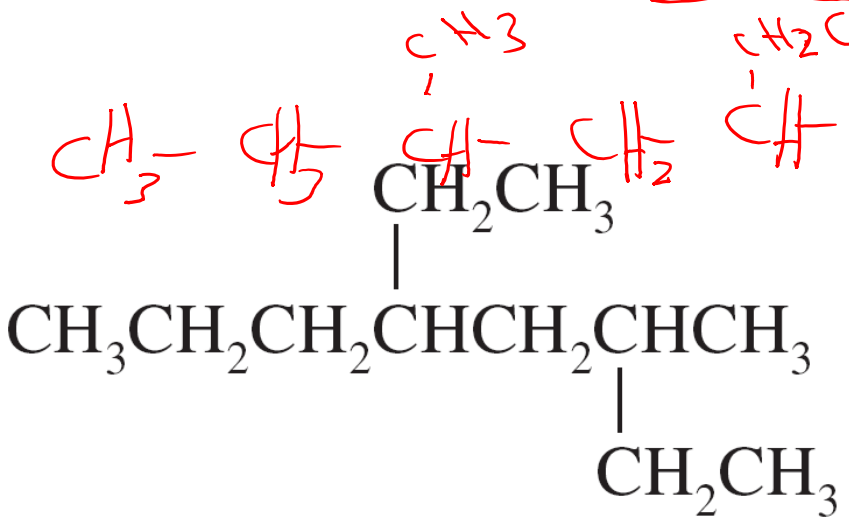
@chem3/phys

Example I. Give the IUPAC name for the this alkane.



2-methylhexane

Example II. Write the formula for 3-methyl-5-ethyloctane.

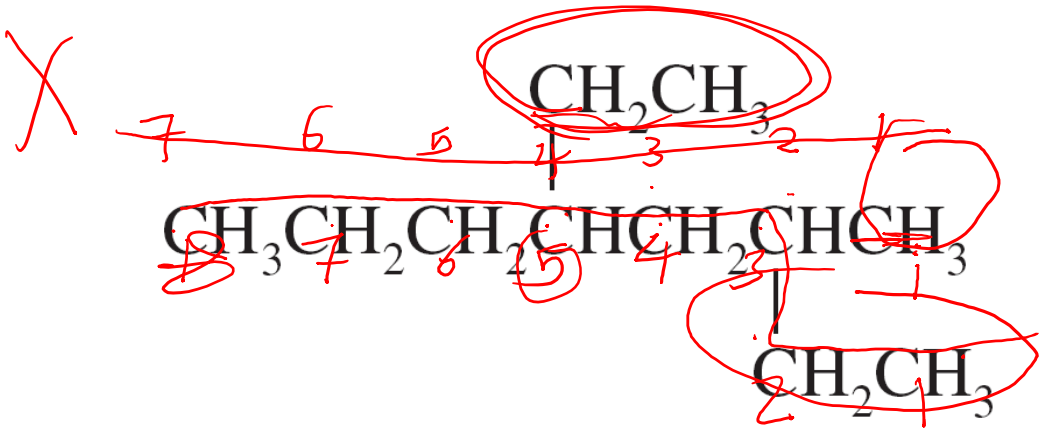


→ 4,6

3,5

3-Methyl – 5-Ethyl octane

X



19.11 Reactions of Alkanes

Combustion

Alkanes are a valuable energy source due to their ability to react with oxygen . Alkanes release a large amount of energy as shown here.

$$CH_4(g) + 2\,O_2(g) \longrightarrow CO_2(g) + 2\,H_2O(g) + 802.5\ kJ\ (191.8\ kcal)$$

$$C_2H_6 + O_2 \longrightarrow CO_2 + H_2O$$

Alkanes generally are considered to be unreactive and for reactions other than combustion a catalyst or other special reaction conditions are necessary.

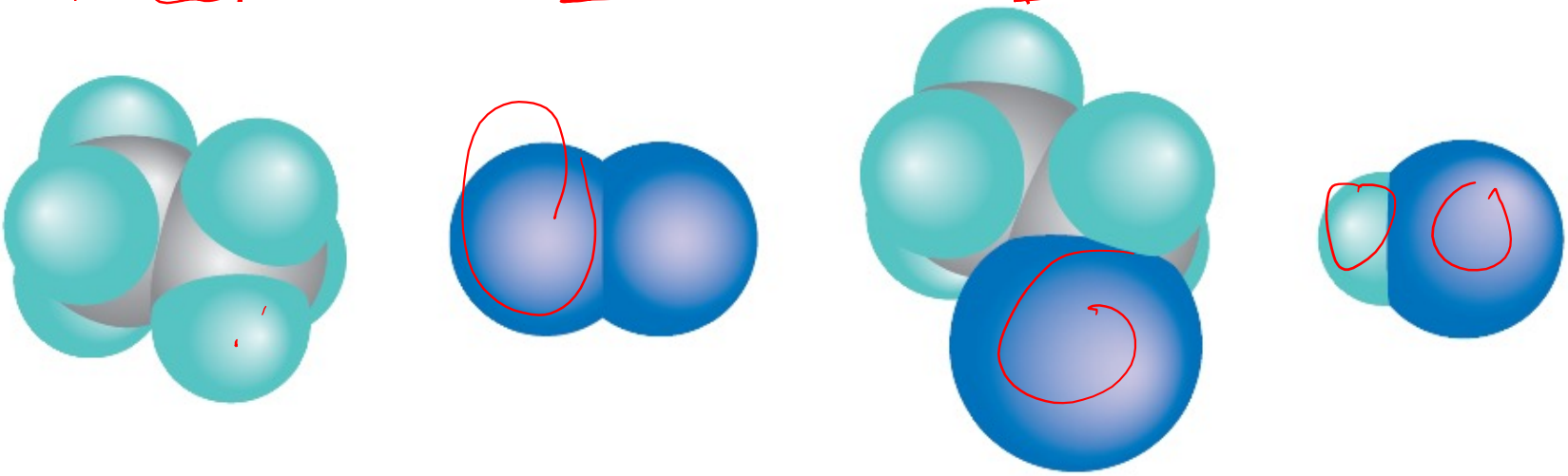
$$CH_4 + Cl_2 \longrightarrow CH_3Cl + HCl$$

$$C_2H_3CH_3 + Cl_2 \longrightarrow CH_3CH_2Cl + HCl$$

Halogenation

Example: $RH + X_2 \longrightarrow RX + HX$ (X = Cl or Br)

$$CH_3CH_3 + Cl_2 \longrightarrow CH_3CH_2Cl + HCl$$



$$CH_4 + Cl_2 \longrightarrow CH_3Cl + HCl$$

$$CH_3Cl + Cl_2 \longrightarrow CH_2Cl_2 + HCl$$

$$CH_2Cl_2 + Cl_2 \longrightarrow \boxed{CHCl_3}$$

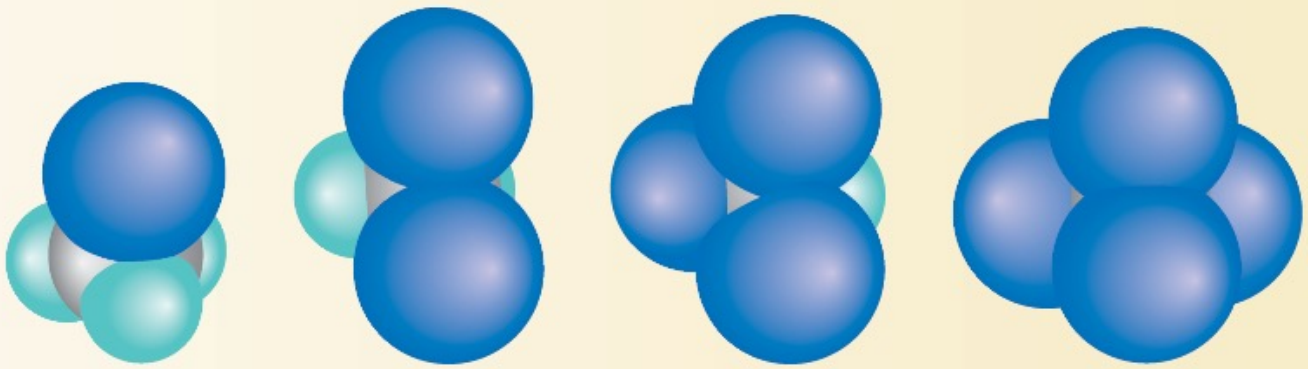
$$CHCl_3 + Cl_2 \longrightarrow CCl_4 + HCl$$

The chlorination of methane can produce each of the compounds shown in Table 19.4.

$$CH_4 \xrightarrow{Cl_2} CH_3Cl \xrightarrow{Cl_2} CH_2Cl_2 \xrightarrow{Cl_2} CHCl_3 \xrightarrow{Cl_2} CCl_4 + 4\,HCl$$

Table 19.4 Chlorination Products of Methane

Formula	IUPAC name	Common name
CH_3Cl	Chloromethane	Methyl chloride
CH_2Cl_2	Dichloromethane	Methylene chloride
$CHCl_3$	Trichloromethane	Chloroform
CCl_4	Tetrachloromethane	Carbon tetrachloride



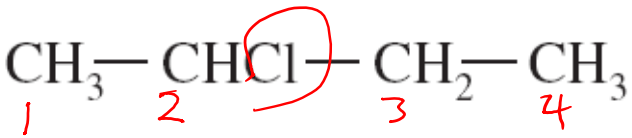
Chloromethane Dichloromethane Trichloromethane Tetrachloromethane

Alkyl Halides

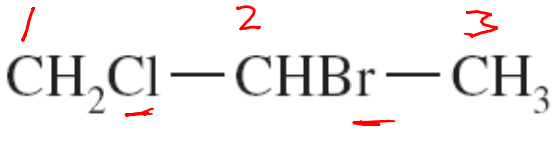
Alkyl halides are compounds that have an X (*X = -F (fluoro), -Cl (chloro), -Br (bromo), or - I (iodo)* attached to a carbon atom.

RX is the general formula for alkyl halides.

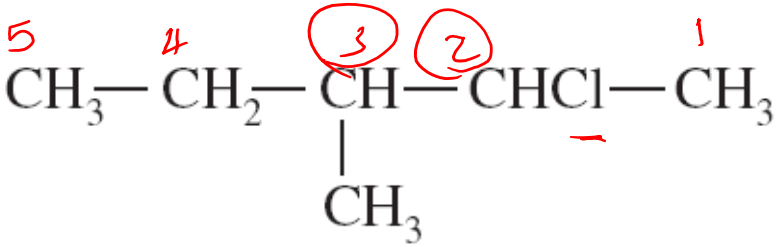
Examples of Alkyl Halides



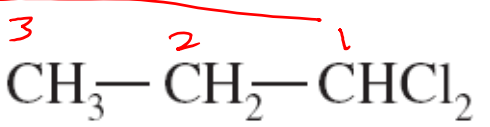
2-chlorobutane



2-bromo-1-chloropropane



2-chloro-3-methylpentane



1,1-dichloropropane

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19.12 Sources of Alkanes

19.13 Gasoline: A Major Petroleum Product

Sources of Alkanes

- Alkanes are produced from natural gas and petroleum.
- Natural gas and petroleum are formed by the decay of plants and animals
- Natural gas and petroleum are non-renewable sources of energy

Gasoline is a major petroleum product

Gasoline is mostly hydrocarbons and without additives it causes knocking which is a detonation of the air-fuel mixture in an engine.

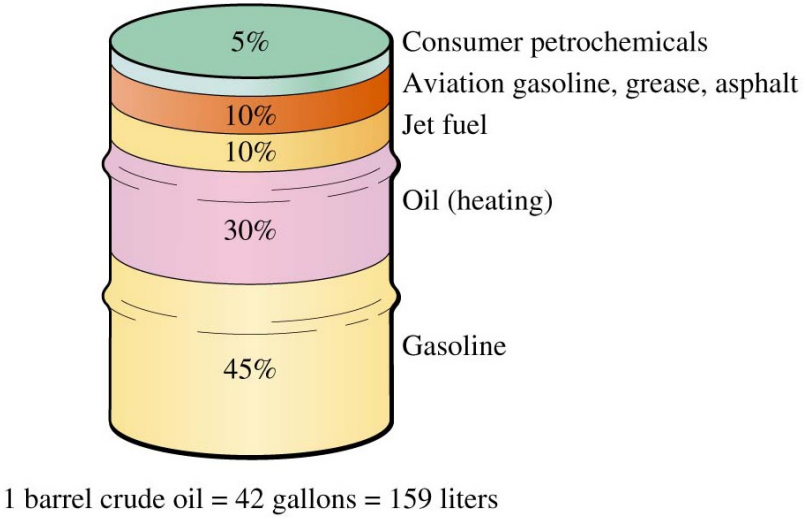


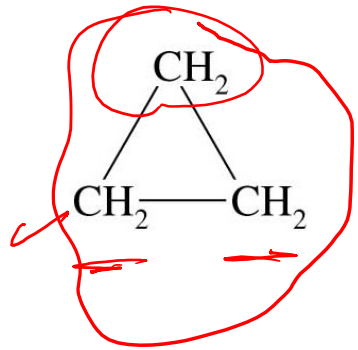
Figure 19.8 Uses of petroleum

The octane rating of gasoline is the knocking performance based on the percent isooctane in an isooctane/heptane mixture. (*higher octane ratings = less knocking)*

19.14 Cycloalkanes

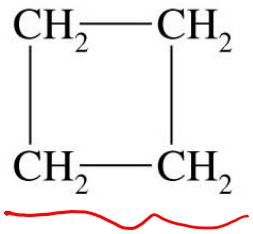
Cycloalkanes

Cycloalkanes are cyclic alkanes with the general formula C_nH_{2n}.



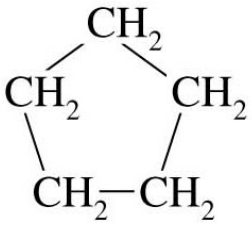
cyclopropane

C_3H_6



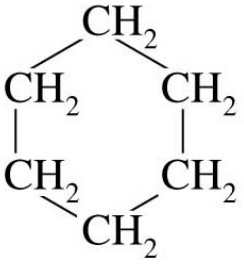
cyclobutane

C_4H_8



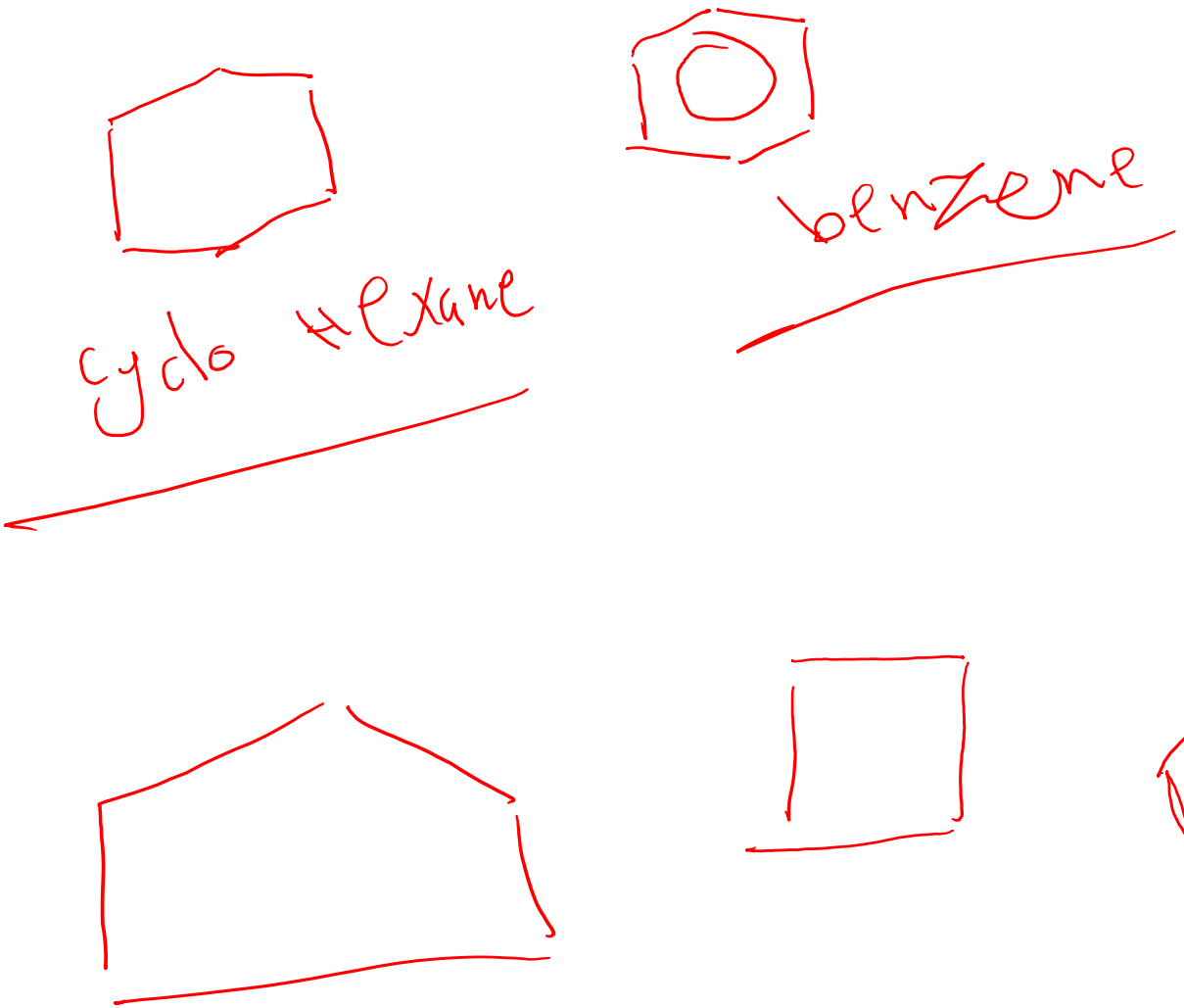
cyclopentane

C_5H_{10}



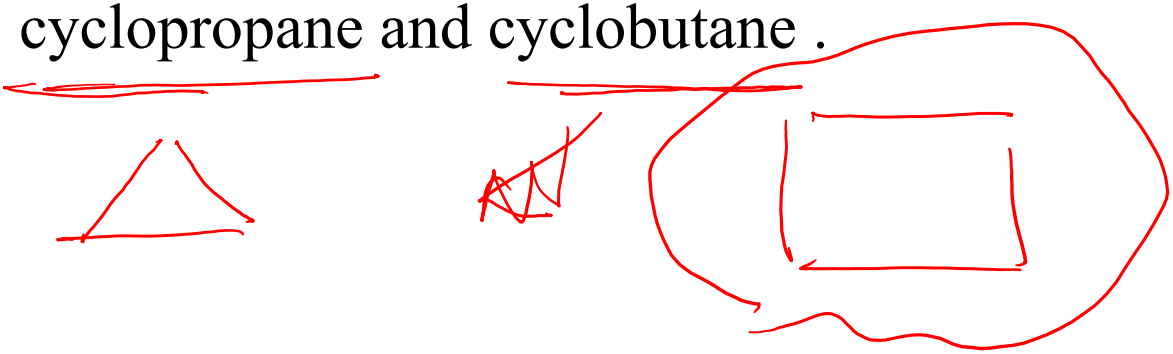
cyclohexane

C_6H_{12}


cyclo hexane
benzene

Properties of Cycloalkanes

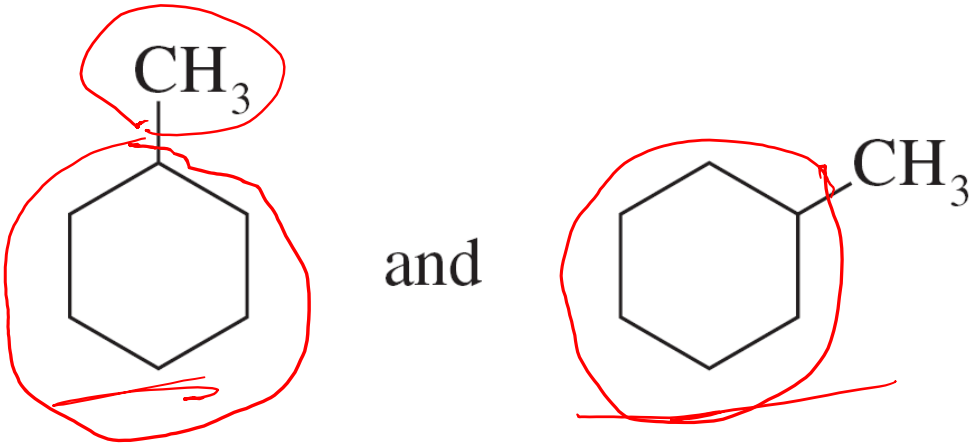
The physical properties and the chemical reactivity of cycloalkanes are similar to their open-chain counterparts with two exceptions: cyclopropane and cyclobutane .



Naming Cycloalkanes

When naming monosubstituted cycloalkanes:

1. Name the substituent
2. Name the parent cyclohexane



Both of these structures are the same molecule and are named this way:

methyl + cyclohexane = methylcyclohexane

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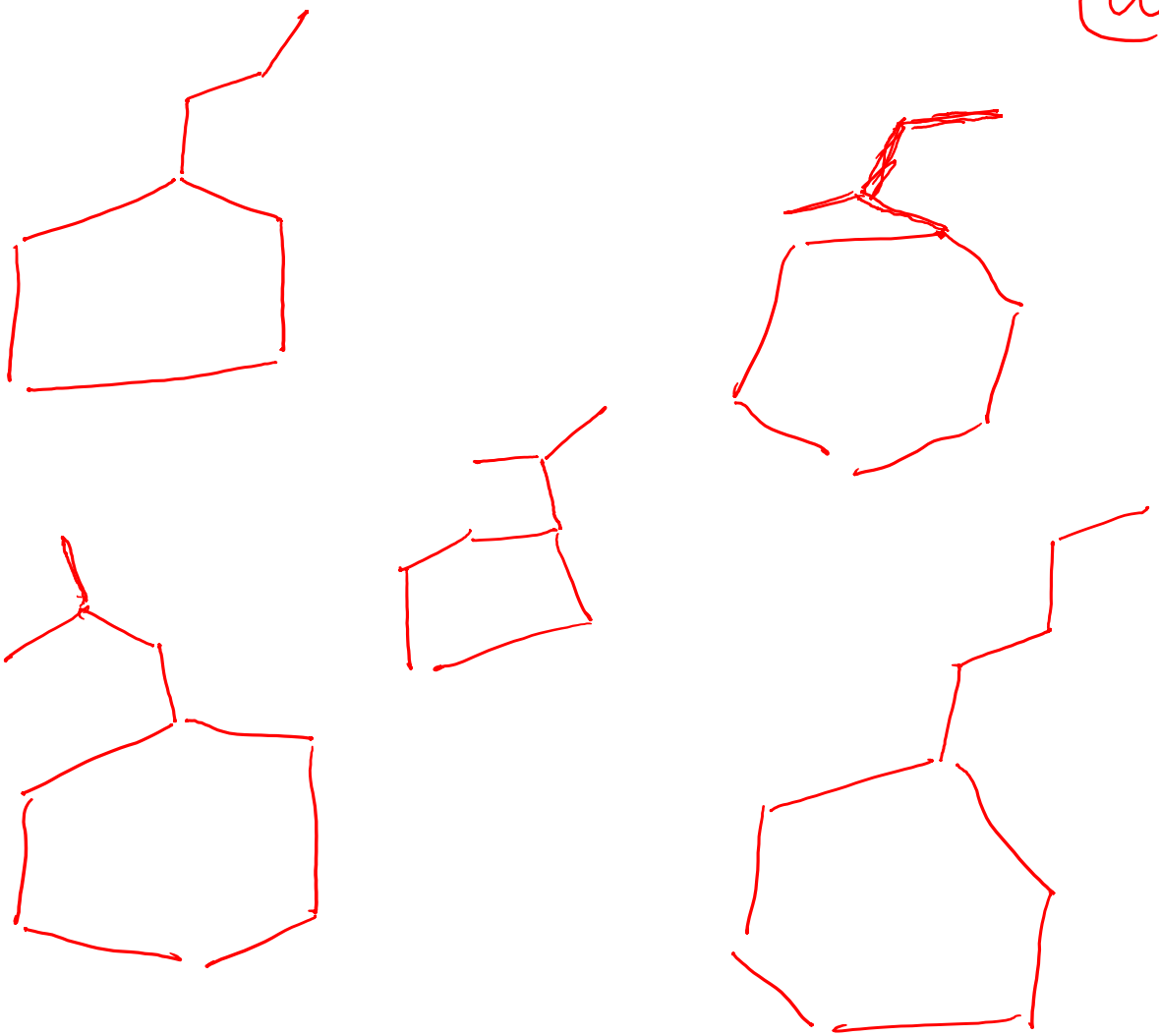
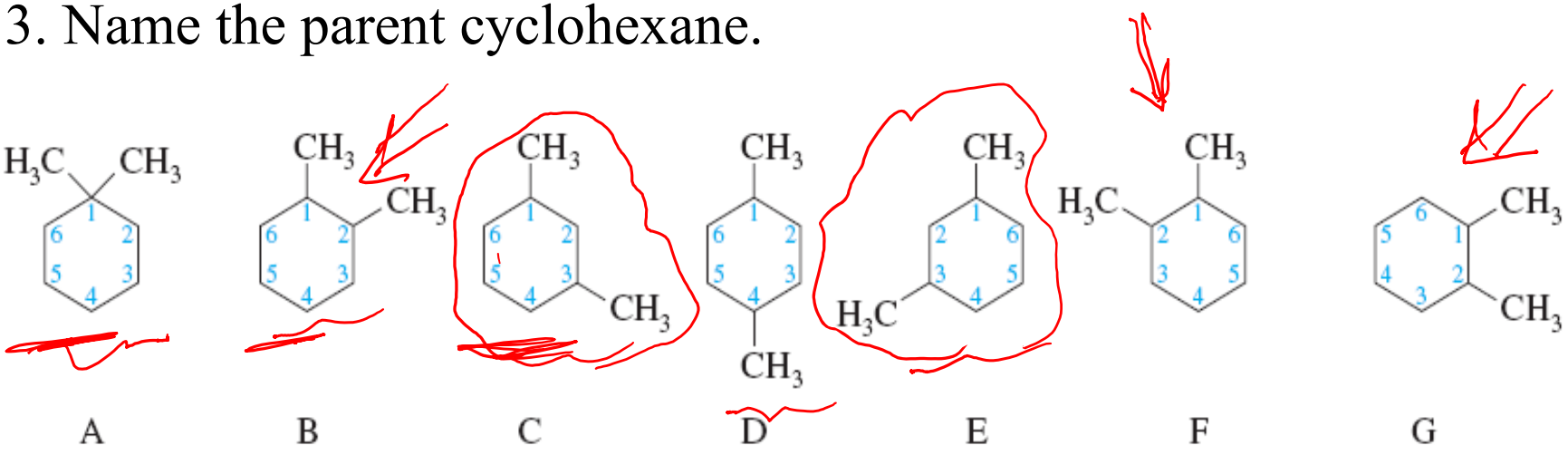


Naming Polysubstituted Cycloalkanes

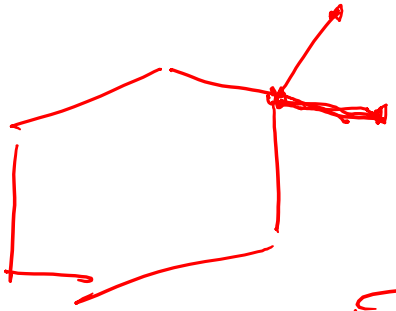
When naming polysubstituted cycloalkanes:

1. Number the ring in a way that gives the smallest total number.
2. Name the substituent and its location.
3. Name the parent cyclohexane.



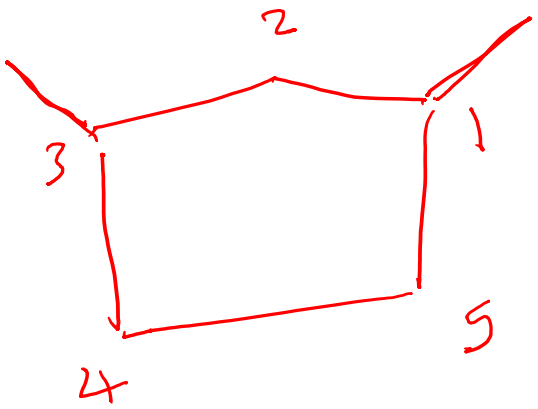
A is 1,1-dimethylcyclohexane
B is 1,2-dimethylcyclohexane
C is 1,3-dimethylcyclohexane
D is 1,4-dimethylcyclohexane

E is 1,3-dimethylcyclohexane (numbered counterclockwise)
F is 1,2-dimethylcyclohexane (numbered counterclockwise)
G is 1,2-dimethylcyclohexane (same as B and F)



1,1-dimethyl

cyclo——————



1,3-dimethyl

cyclopentane

Chapter 19 Summary

- Organic chemistry is the chemistry of carbon compounds.

- Alkanes are hydrocarbons that are either saturated *(no double or triple bonds)* or unsaturated *(one or more multiple bonds)*.

- Organic compounds are classified by functional groups which is the smaller part of the molecule that determines the chemical profile of the molecule.

- Organic molecules can be represented by ball-and stick models, space-filling models, Lewis structures, line structures , and condensed structural formulas.

- Saturated carbon atoms are sp^3 hybridized which form can four sigma bonds .

Chapter 19 Summary

- Reactions of organic molecules are classified as substitution, elimination, and addition.

- Alkanes undergo combustion but need special reaction conditions to undergo halogenation, dehydrogenation, cracking, and isomerization.

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