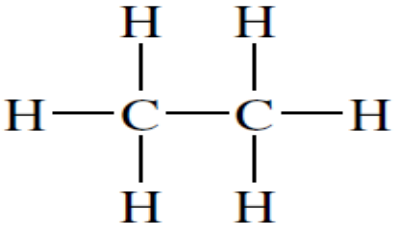
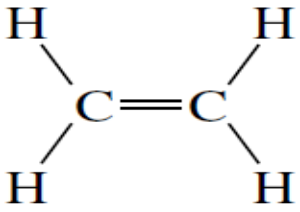
Alkanes

Hydrocarbons: 1. Aliphatic 2. Aromatic

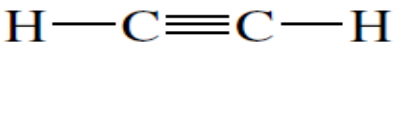
Alkanes; Alkenes; Alkynes; Arenes



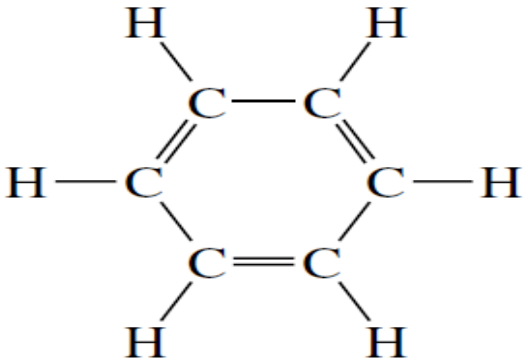
Ethane
(alkane)



Ethylene
(alkene)



Acetylene
(alkyne)



Benzene
(arene)

- **Alkanes**

They Contain: Hydrogen, Carbon; Single bond; SP^3 Carbon; Least reactive compounds; No reactive functional groups; Saturated hydrocarbon; No electrophile; No neocleophile; C_nH_{2n+2} Structures.

- **Alkenes**

They Contain: Hydrogen, Carbon; Double bond; SP^2 Carbon; Unsaturated hydrocarbon; C_nH_{2n} Structures.

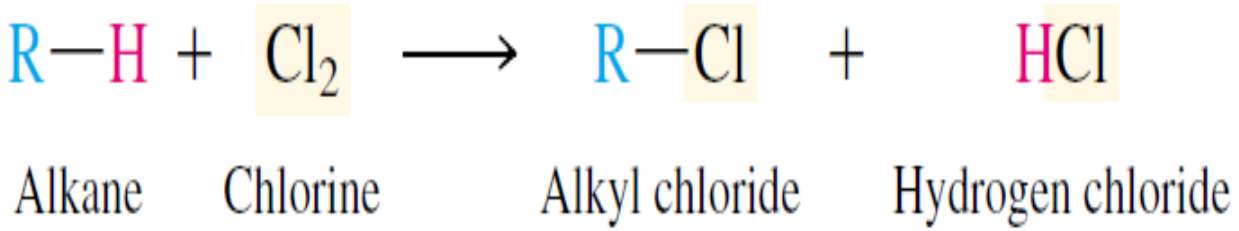
- **Alkynes**

They Contain: Hydrogen, Carbon; Triple bond; SP Carbon; Unsaturated hydrocarbon; C_nH_{2n-2} Structures.

- **Cyclic hydrocarbons**

They Contain: Hydrogen, Carbon; Single bond; SP^3 Carbon; Cyclic structure; C_nH_{2n} Structures.

- The family of organic compounds
- Functional groups: R-Cl, R-CN, R-OH, R-CHO, R-NH_2, R-O-R, R-NO_2, R-SH
- Reactive sides of hydrocarbons



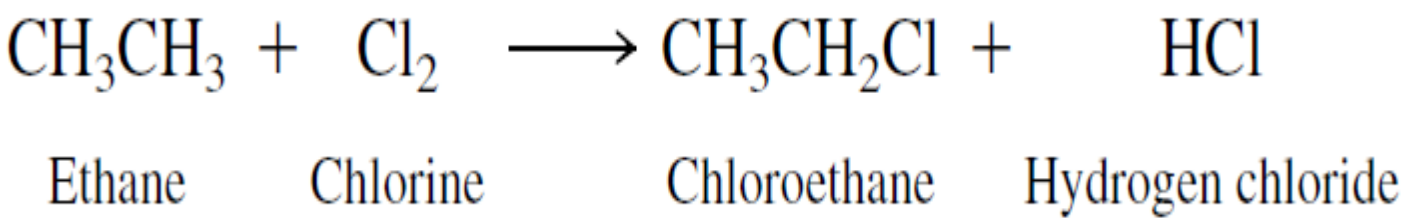
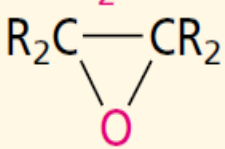
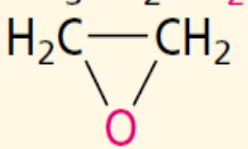
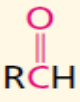
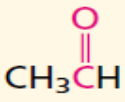
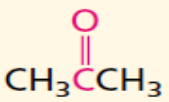
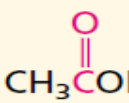
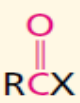
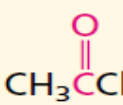
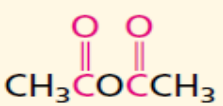
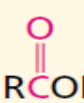
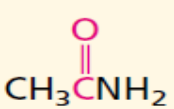


TABLE 2.1 Functional Groups in Some Important Classes of Organic Compounds

Class	Generalized abbreviation	Representative example	Name of example*
Alcohol	ROH	CH_3CH_2OH	Ethanol
Alkyl halide	RCl	CH_3CH_2Cl	Chloroethane
Amine†	RNH_2	$CH_3CH_2NH_2$	Ethanamine
Epoxide			Oxirane
Ether	ROR	$CH_3CH_2OCH_2CH_3$	Diethyl ether
Nitrile	$RC{\equiv}N$	$CH_3CH_2C{\equiv}N$	Propanenitrile
Nitroalkane	RNO_2	$CH_3CH_2NO_2$	Nitroethane
Thiol	RSH	CH_3CH_2SH	Ethanethiol

*Most compounds have more than one acceptable name.
†The example given is a *primary* amine (RNH_2). *Secondary* amines have the general structure R_2NH; *tertiary* amines are R_3N.

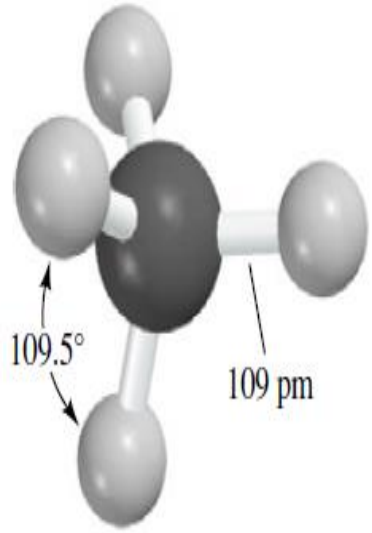
TABLE 2.2 Classes of Compounds That Contain a Carbonyl Group

Class	Generalized abbreviation	Representative example	Name of example
Aldehyde			Ethanal
Ketone			2-Propanone
Carboxylic acid			Ethanoic acid
Carboxylic acid derivatives:			
Acyl halide			Ethanoyl chloride
Acid anhydride			Ethanoic anhydride
Ester			Ethyl ethanoate
Amide			Ethanamide

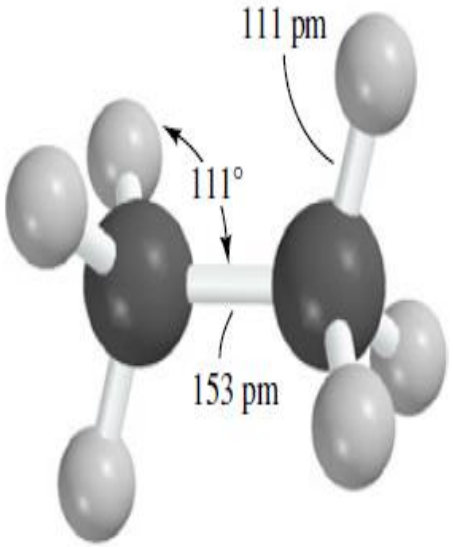
Nomenclature

1. Common names; 2. The IUPAC names

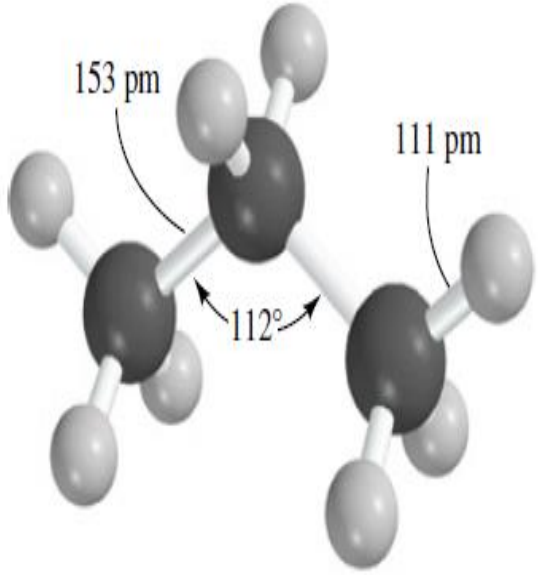
Methane; Ethane; Propane



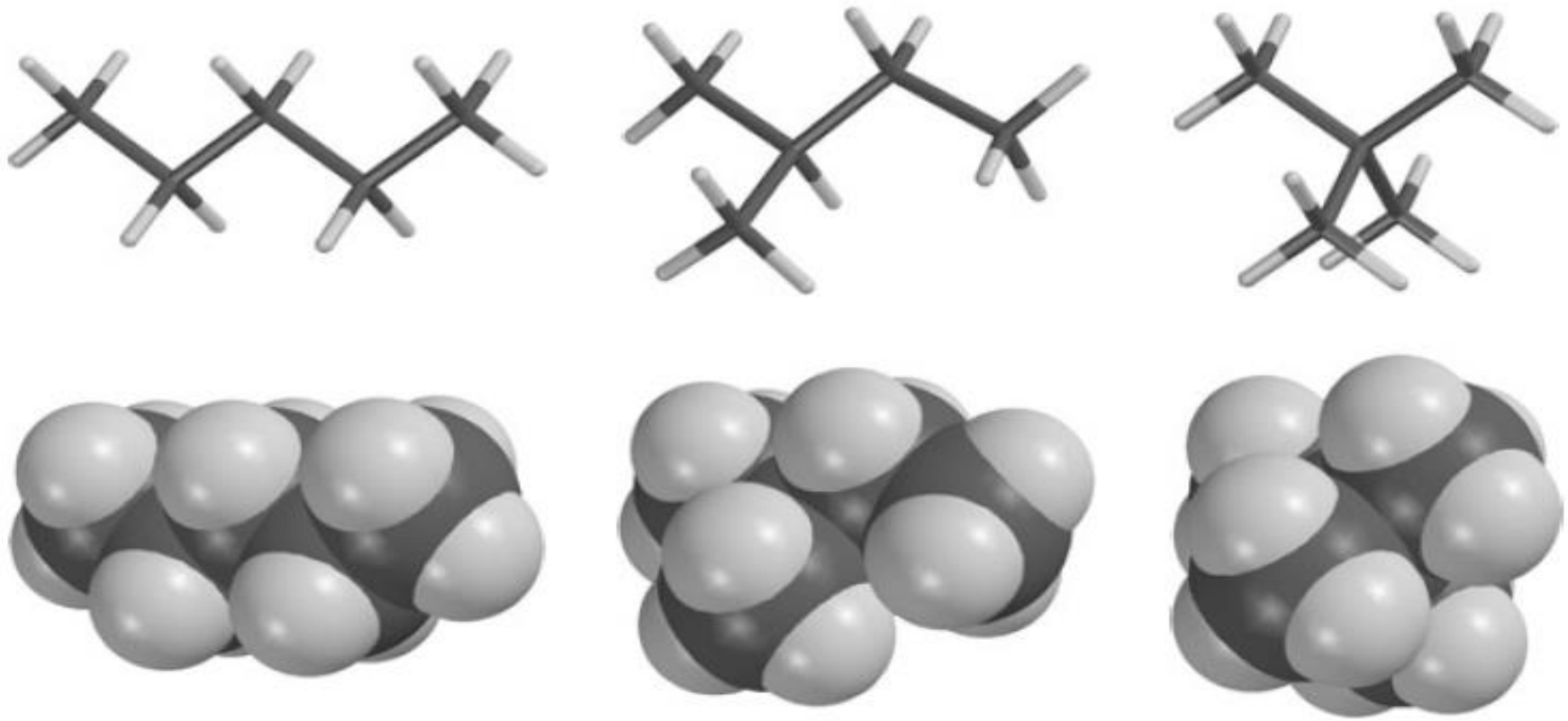
Methane



Ethane



Propane



(*a*) Pentane: $CH_3CH_2CH_2CH_2CH_3$

(*b*) 2-Methylbutane: $(CH_3)_2CHCH_2CH_3$

(*c*) 2,2-Dimethylpropane: $(CH_3)_4C$

FIGURE 2.4 Space-filling models of (*a*) pentane, (*b*) 2-methylbutane, and (c) 2,2-dimethylpropane. The most branched isomer, 2,2-dimethylpropane, has the most compact, most spherical, three-dimensional shape.

Properties

	CH_4	CH_3CH_3	$CH_3CH_2CH_3$	$CH_3CH_2CH_2CH_2CH_3$	$CH_3CH(CH_3)CH_2CH_3$	$CH_3C(CH_3)_2CH_3$
	Methane	Ethane	Propane	Pentane	2-Methylbutane	2,2-Dimethylpropane
Boiling point:	−160°C	−89°C	−42°C	(bp 36°C)	(bp 28°C)	(bp 9°C)

Intermolecular forces (Induced dipole interaction)

Van der Waals forces (London forces)

Each additional $–CH_2-$ group increases the boiling point by about 30 °C up to about ten carbons, and by about 20 °C in higher alkanes.

Solubility in water: Insoluble

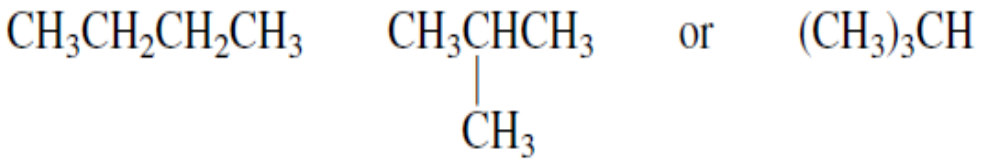
Hydrophobic (water hating)

Alkane density: about 0.7 g/ml

	CH_4	CH_3CH_3	$CH_3CH_2CH_3$
	Methane	Ethane	Propane
Boiling point:	−160°C	−89°C	−42°C

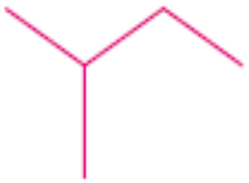
Isomeric alkanes:

1. Constitutional isomer
2. 2. Stereoisomers



	n-Butane	Isobutane
Boiling point:	−0.4°C	−10.2°C
Melting point:	−139°C	−160.9°C

n-Pentane: $CH_3CH_2CH_2CH_2CH_3$ or $CH_3(CH_2)_3CH_3$ or 

Isopentane: $CH_3CHCH_2CH_3$ (with CH_3 branch) or $(CH_3)_2CHCH_2CH_3$ or 

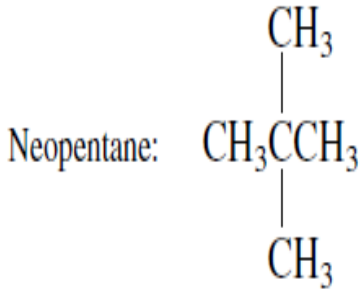
Neopentane:  or $(CH_3)_4C$ or 

TABLE 2.3 The Number of Constitutionally Isomeric Alkanes of Particular Molecular Formulas

Molecular formula	Number of constitutional isomers
CH_4	1
C_2H_6	1
C_3H_8	1
C_4H_{10}	2
C_5H_{12}	3
C_6H_{14}	5
C_7H_{16}	9
C_8H_{18}	18
C_9H_{20}	35
$C_{10}H_{22}$	75
$C_{15}H_{32}$	4,347
$C_{20}H_{42}$	366,319
$C_{40}H_{82}$	62,491,178,805,831

TABLE 2.4 IUPAC Names of Unbranched Alkanes

Number of carbon atoms	Name	Number of carbon atoms	Name	Number of carbon atoms	Name
1	Methane	11	Undecane	21	Henicosane
2	Ethane	12	Dodecane	22	Docosane
3	Propane	13	Tridecane	23	Tricosane
4	Butane	14	Tetradecane	24	Tetracosane
5	Pentane	15	Pentadecane	30	Triacontane
6	Hexane	16	Hexadecane	31	Hentriacontane
7	Heptane	17	Heptadecane	32	Dotriacontane
8	Octane	18	Octadecane	40	Tetracontane
9	Nonane	19	Nonadecane	50	Pentacontane
10	Decane	20	Icosane*	100	Hectane

*Spelled "eicosane" prior to 1979 version of IUPAC rules.

A homologous series: Series unbranched alkanes that differ only by the number of -CH_2- groups.

$CH_3CH_2CH_2CH_2CH_2CH_3$

IUPAC name: hexane

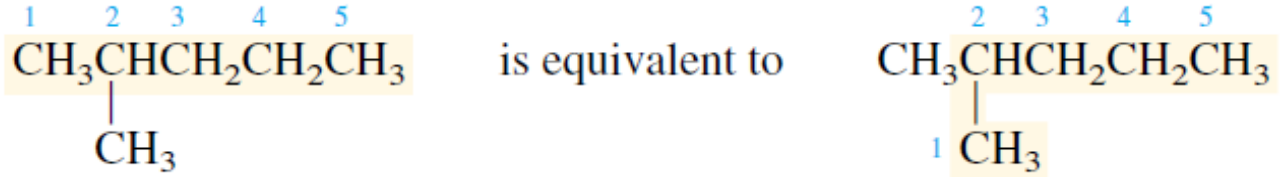
(common name: *n*-hexane)

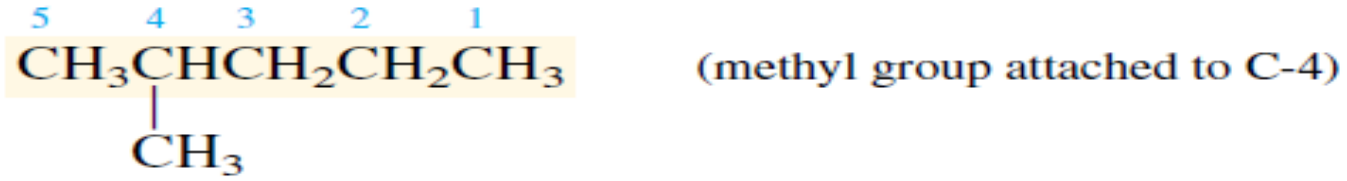
1. Longest continuous chain
2. Identify the substituent group
3. Give the lowest number to the substituent
4. Write the name of compound

Name the substituent groups attached to the longest chain as **alkyl groups.**

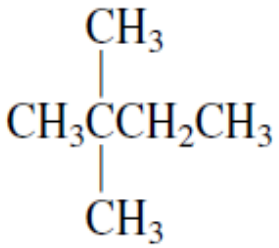
Alkyl groups: Methyl; Ethyl; n-Propyl

CH_3-; CH_3-CH_2-; CH_3-CH_2-CH_2-

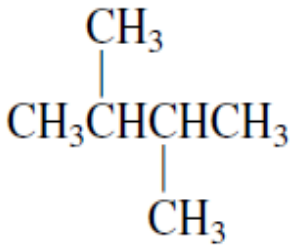




(methyl group attached to C-4)

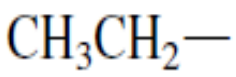


IUPAC name: 2,2-dimethylbutane

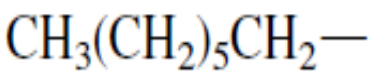


IUPAC name: 2,3-dimethylbutane

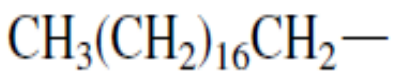
Alkyl group:



Ethyl group

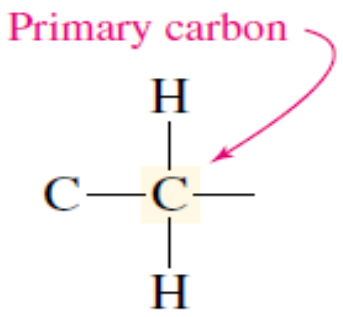


Heptyl group

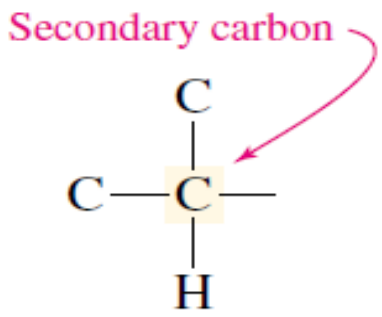


Octadecyl group

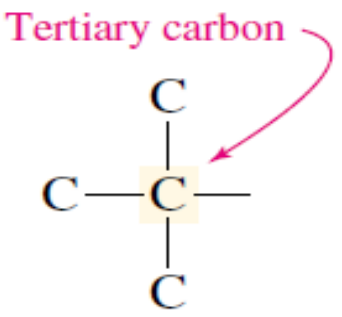
Classification



Primary alkyl group



Secondary alkyl group



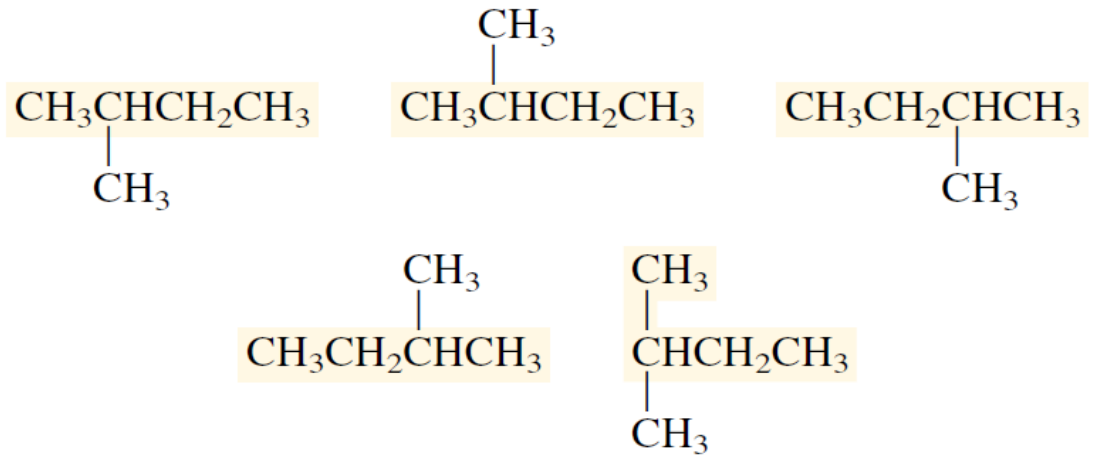
Tertiary alkyl group

- When there are two longest chains of equal length, use the chain with the greater number of substituents as the main chain.

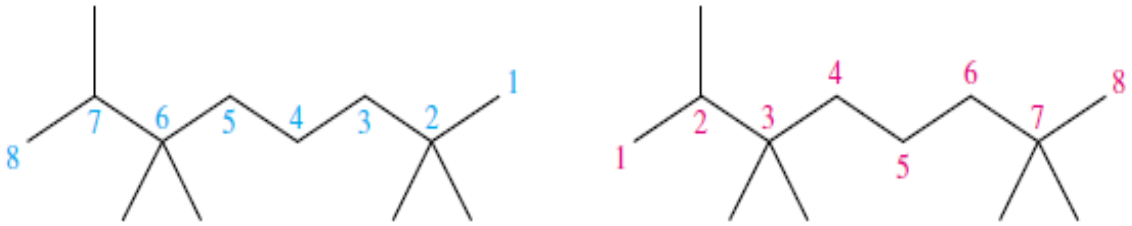
- The longest chain, beginning with the end of name the substituent groups attached to the longest the chain nearest a substituent.

- Give the location of each alkyl group by the number of the main-chain carbon atom to which it is attached.

- $-CH_3$ Methyl unit or group; $-CH_2-$ Methylene group; -CH Methine group



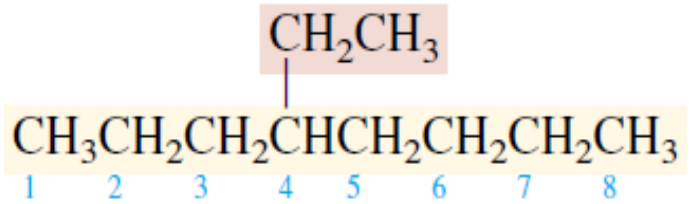
The same compounds



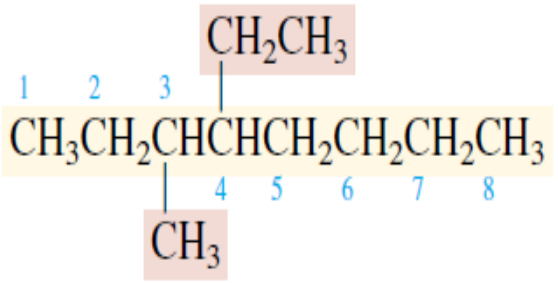
2,2,6,6,7-Pentamethyloctane
(correct)

2,3,3,7,7-Pentamethyloctane
(incorrect!)

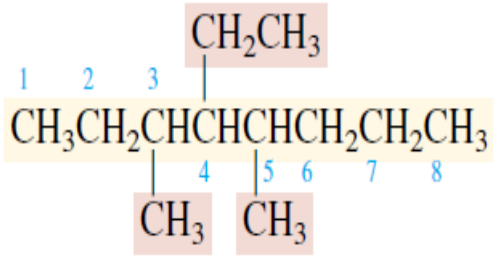
Bond line formula



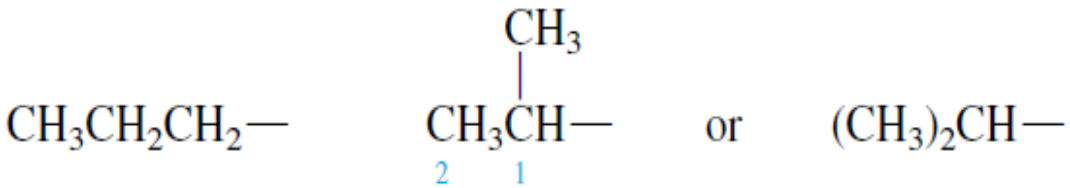
4-ethyloctane



4-ethyl-3-methyloctane

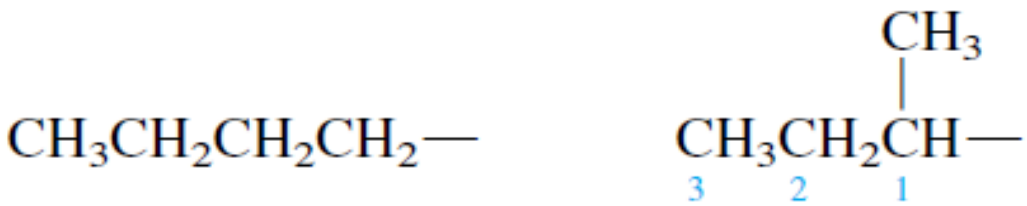


4-ethyl-3,5-dimethyloctane



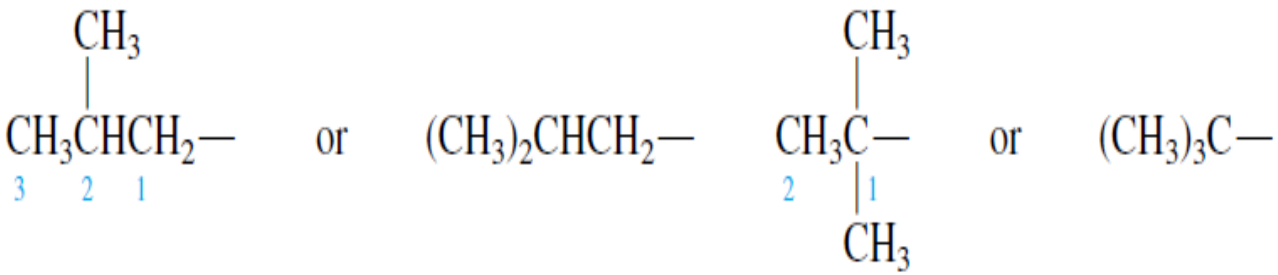
Propyl group
(common name: *n*-propyl)

1-Methylethyl group
(common name: isopropyl)



Butyl group
(common name: *n*-butyl)

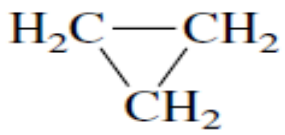
1-Methylpropyl group
(common name: *sec*-butyl)



2-Methylpropyl group
(common name: isobutyl)

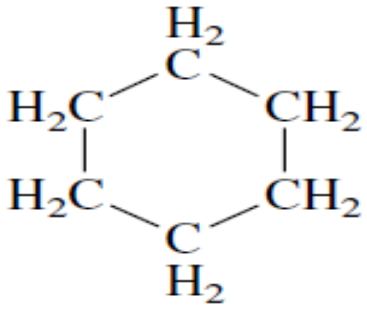
1,1-Dimethylethyl group
(common name: *tert*-butyl)

Cycloalkanes:

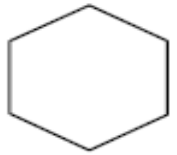


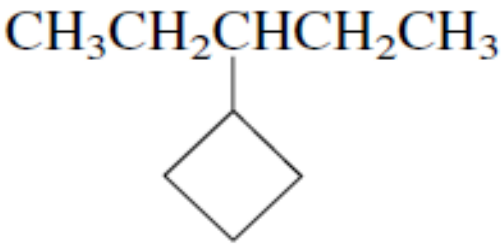
Cyclopropane

usually represented as 

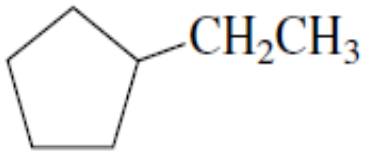


Cyclohexane

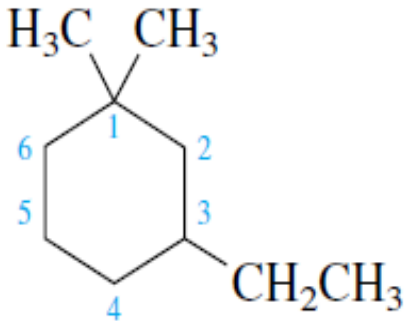
usually represented as 



3-Cyclobutylpentane



Ethylcyclopentane



3-Ethyl-1,1-dimethylcyclohexane
(not 1-ethyl-3,3-dimethylcyclohexane, because first point of difference rule requires 1,1,3 substitution pattern rather than 1,3,3)

Distilation

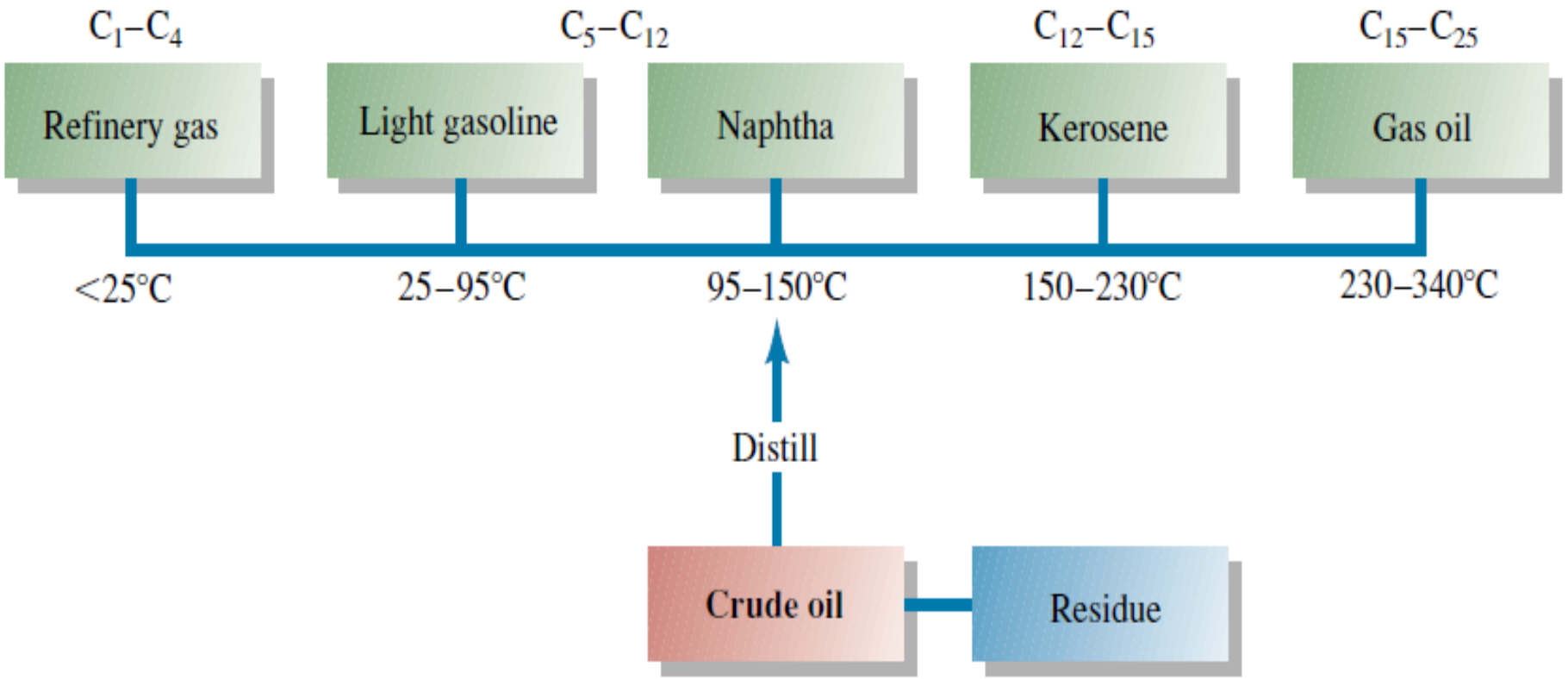
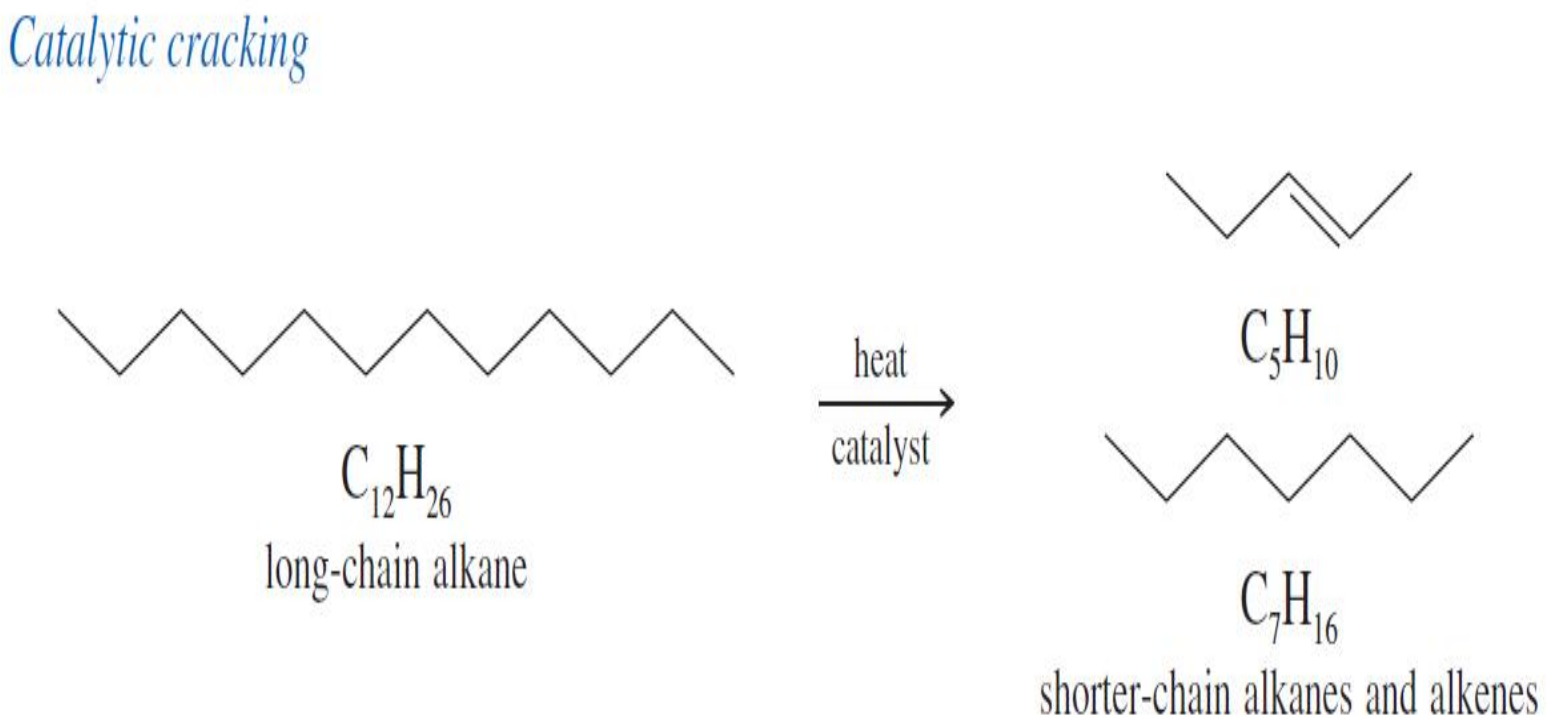


FIGURE 2.2 Distillation of crude oil yields a series of volatile fractions having the names indicated, along wih a nonvolatile residue. The number of carbon atoms that characterize the hydrocarbons in each fraction is approximate.

Reactions

Cracking: Conversions of large alkane molecules to small alkane molecules.



Reforming: Conversion of alkanes to highly branched alkanes and aromatic compounds.

TABLE 3-3 Major Fractions Obtained from Distillation of Crude Petroleum

Boiling Range (°C)	Number of Carbons	Fraction	Use
under 30°	2–4	petroleum gas	LP gas for heating
30°–180°	4–9	gasoline	motor fuel
160°–230°	8–16	kerosene	heating, jet fuel
200°–320°	10–18	diesel	motor fuel
300°–450°	16–30	heavy oil	heating, lubrication
>300° (vacuum)	>25	petroleum "jelly,"	
		paraffin "wax"	
residue	>35	asphalt	

Combustion

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O \qquad \Delta H^\circ = -890\ \text{kJ}\ (-212.8\ \text{kcal})$$

Methane Oxygen Carbon dioxide Water

$$(CH_3)_2CHCH_2CH_3 + 8O_2 \longrightarrow 5CO_2 + 6H_2O \qquad \Delta H^\circ = -3529\ \text{kJ}\ (-843.4\ \text{kcal})$$

2-Methylbutane Oxygen Carbon dioxide Water

$\Delta H^o = H^o_{Products} - H^o_{Reactants}$

H^o = The heat content or Enthalpy

In exothermic reaction: $\Delta H^o = - \quad H^o_{Products} < H^o_{Reactants}$

In endxothermic reaction: $\Delta H^o = + \quad H^o_{Products} > H^o_{Reactants}$

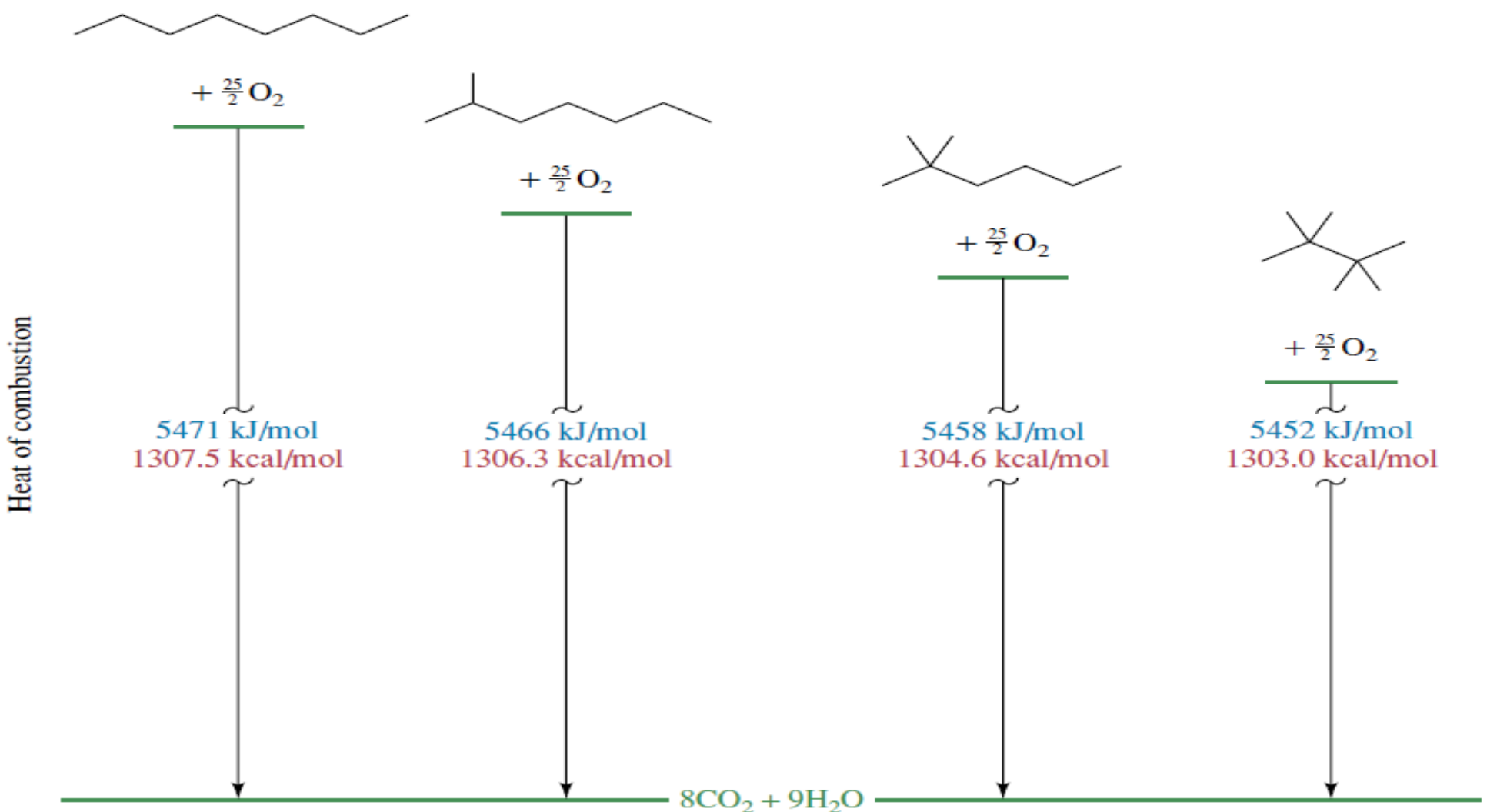
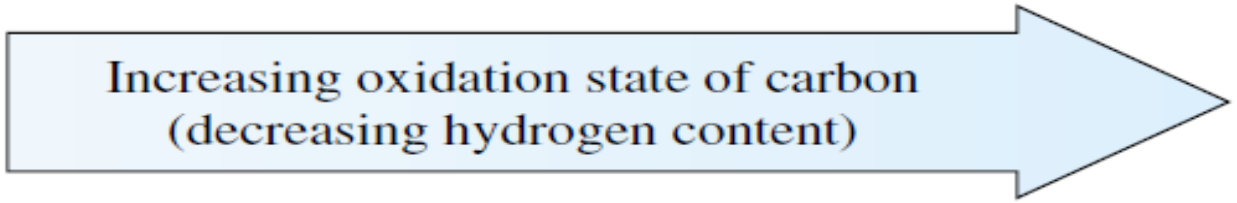


FIGURE 2.5 Energy diagram comparing heats of combustion of isomeric C_8H_{18} alkanes.



CH_3CH_3	$CH_2{=}CH_2$	$HC{\equiv}CH$
Ethane	Ethylene	Acetylene
(6 C—H bonds)	(4 C—H bonds)	(2 C—H bonds)

Oxidation reactions:

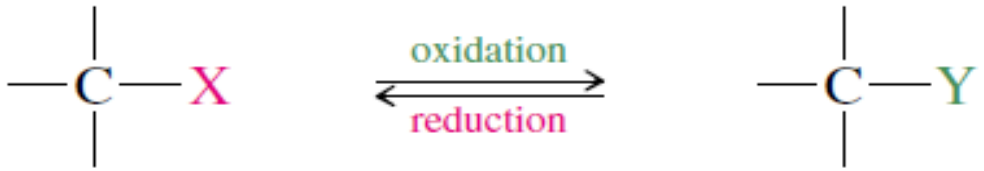
$$CH_4 + Cl_2 \longrightarrow CH_3Cl + HCl$$

Methane + Chlorine → Chloromethane + Hydrogen chloride

Reduction:

$$CH_3Cl + 2Li \longrightarrow CH_3Li + LiCl$$

Chloromethane + Lithium → Methyllithium + Lithium chloride



X is less electronegative than carbon

Y is more electronegative than carbon

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

Ethane Chlorine Chloroethane Hydrogen chloride

$$R{-}H + Cl_2 \longrightarrow R{-}Cl + HCl$$

Alkane Chlorine Alkyl chloride Hydrogen chloride