

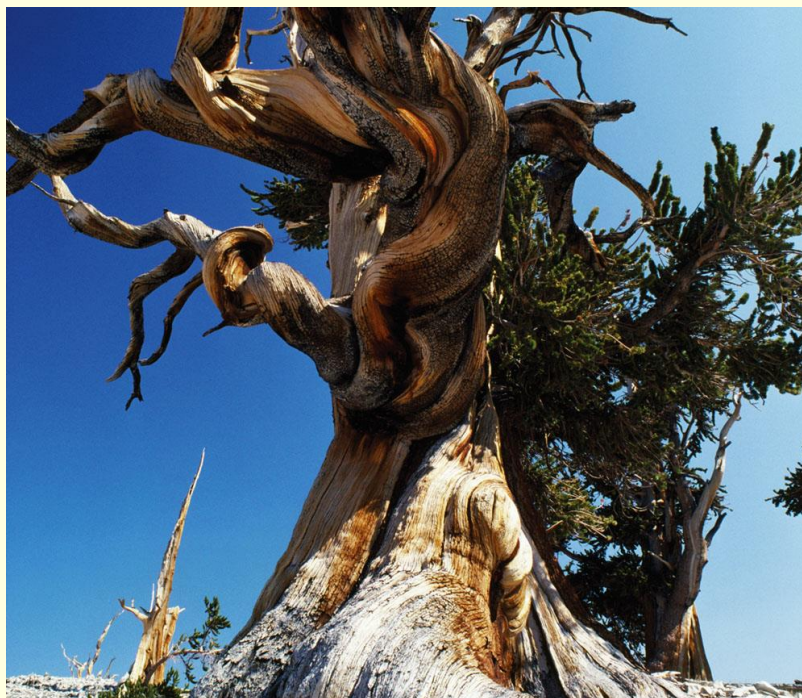


2. Alkanes: The Nature of Organic Compounds

스마트헬스케어학부 의공학전공

임해균 교수

2. Alkanes: The Nature of Organic Compounds



Why this Chapter

- Alkanes are unreactive, because they are rarely involved in chemical reactions. However, they introduce important ideas about organic compounds
- Alkanes will be used to discuss basic approaches to **naming organic compounds**
- We will take an initial look at 3-D aspects of molecules

2.1 Functional Groups

- **Functional group** - collection of atoms at a site that **have a characteristic behavior** in all molecules where it occurs
- For example, the double bonds in simple and complex alkenes react **with bromine** in the same way

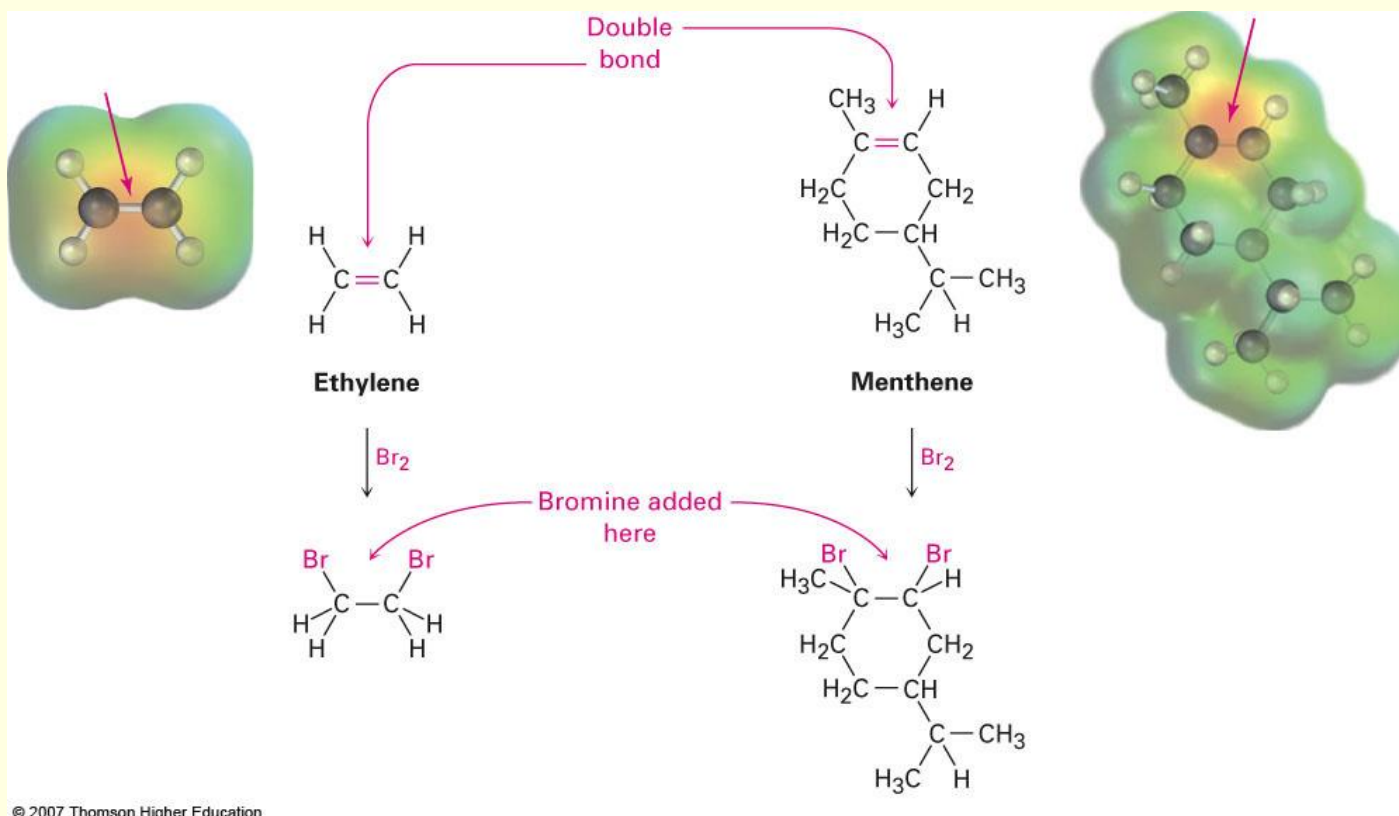

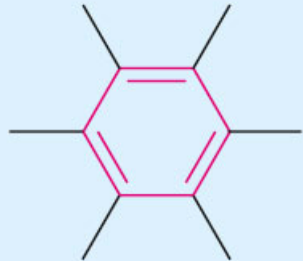



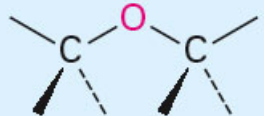
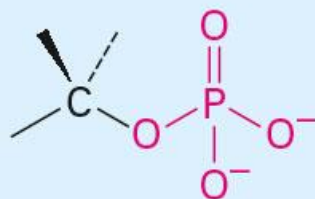


Table 2.1
Structure of Some Common Functional Groups

Name	Structure*	Name ending	Example
Alkene (double bond)		-ene	$\text{H}_2\text{C}=\text{CH}_2$ Ethene
Alkyne (triple bond)	$-\text{C}\equiv\text{C}-$	-yne	$\text{HC}\equiv\text{CH}$ Ethyne
Arene (aromatic ring)		None	 Benzene
Halide	 (X = F, Cl, Br, I)	None	CH_3Cl <div>Chloromethane</div>
Alcohol		-ol	CH_3OH Methanol
Ether		ether	CH_3OCH_3 Dimethyl ether

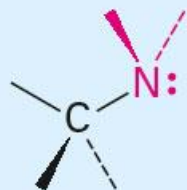
Monophosphate



phosphate

$\text{CH}_3\text{OPO}_3^{2-}$
Methyl phosphate

Amine



-amine

CH_3NH_2
Methylamine

Imine
(Schiff base)



None

$\text{CH}_3\text{C}(\text{CH}_3)=\text{NH}$
Acetone imine

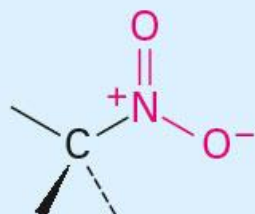
Nitrile



-nitrile

$\text{CH}_3\text{C}\equiv\text{N}$
Ethanenitrile

Nitro



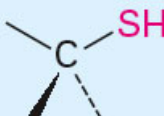
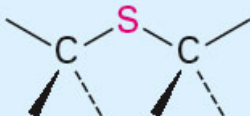
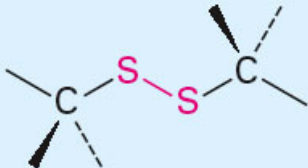
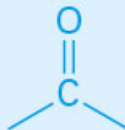
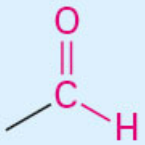
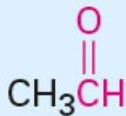
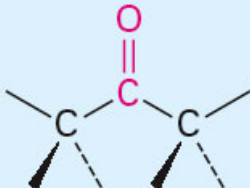
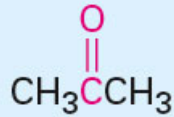
None

CH_3NO_2
Nitromethane

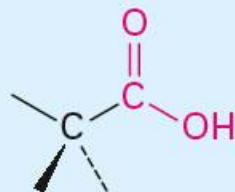
*The bonds whose connections aren't specified are assumed to be attached to carbon or hydrogen atoms in the rest of the molecule.

Table 2.1

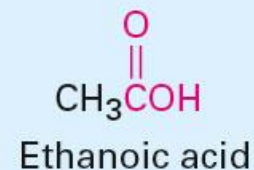
Structure of Some Common Functional Groups (*continued*)

Name	Structure*	Name ending	Example
Thiol		<i>-thiol</i>	CH ₃ SH Methanethiol
Sulfide		<i>sulfide</i>	CH ₃ SCH ₃ Dimethyl sulfide
Disulfide		<i>disulfide</i>	CH ₃ SSCH ₃ Dimethyl disulfide
Carbonyl			
Aldehyde		<div>-al</div>	 Ethanal
Ketone		<div>-one</div>	 Propanone

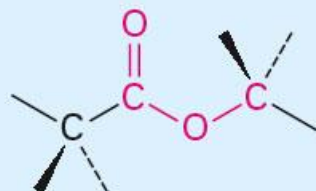
Carboxylic acid



-oic acid



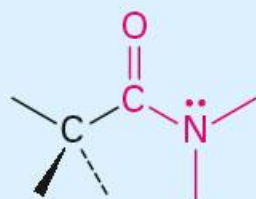
Ester



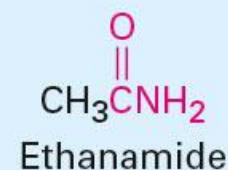
-oate



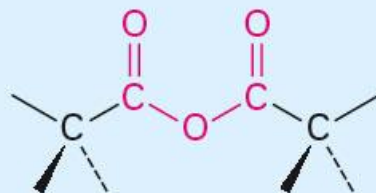
Amide



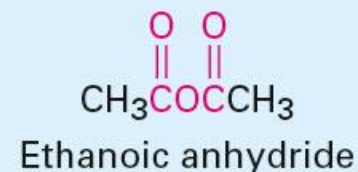
-amide



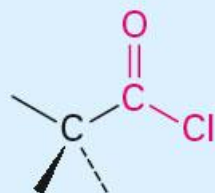
Carboxylic acid
anhydride



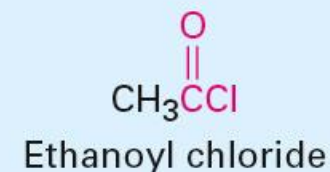
-oic anhydride



Carboxylic acid
chloride



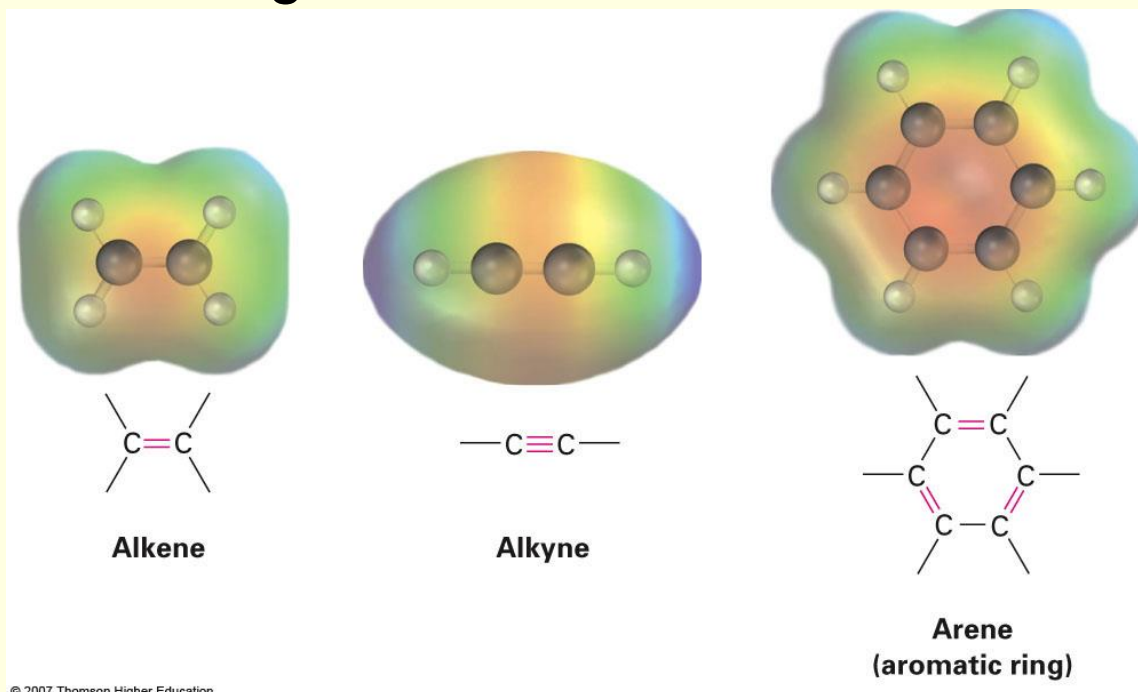
-oyl chloride



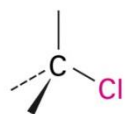
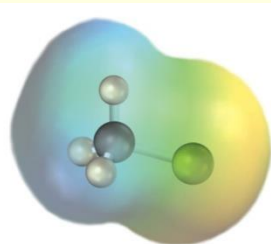
*The bonds whose connections aren't specified are assumed to be attached to carbon or hydrogen atoms in the rest of the molecule.

Functional Groups with Carbon–Carbon Multiple Bonds

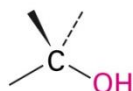
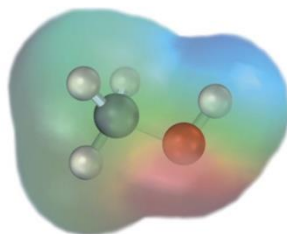
- **Alkenes** have a C-C double bond
- **Alkynes** have a C-C triple bond
- **Arenes** have special bonds that are represented as alternating single and double C-C bonds in a six-membered ring



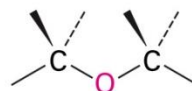
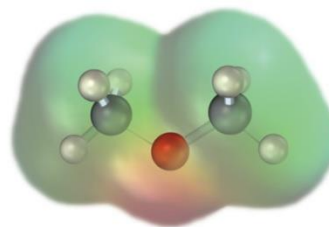
Functional Groups with **Carbon Singly Bonded** to an Electronegative Atom



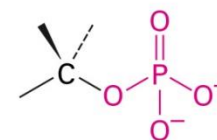
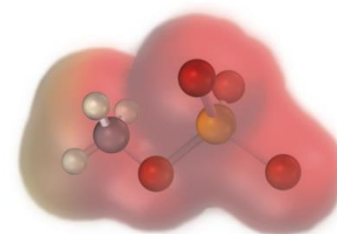
**Alkyl halide
(haloalkane)**



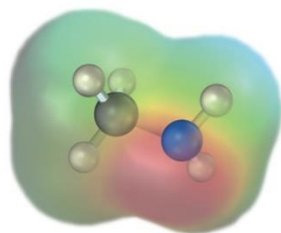
Alcohol



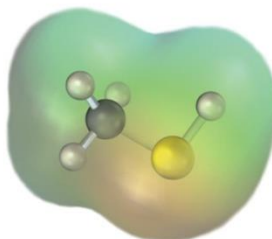
Ether



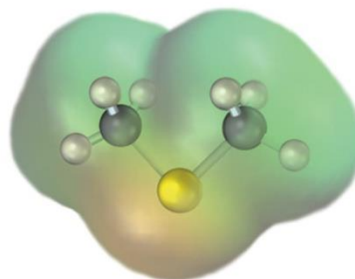
Phosphate



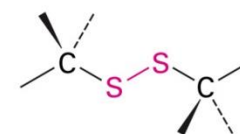
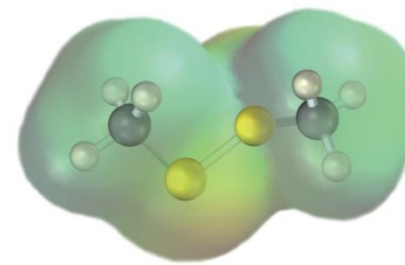
Amine



Thiol

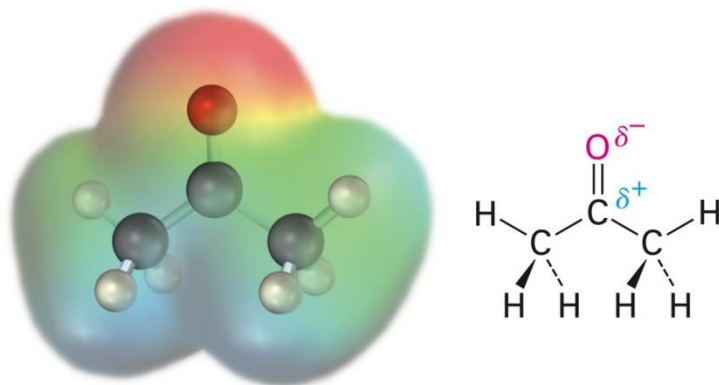


Sulfide

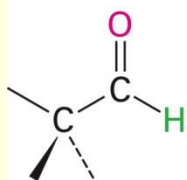


Disulfide

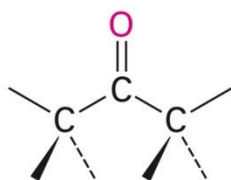
Functional Groups with a Carbon–Oxygen Double Bond (Carbonyl Groups)



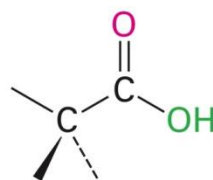
Acetone—a typical carbonyl compound



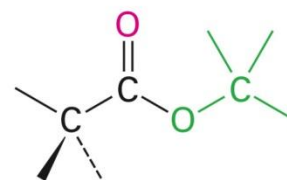
Aldehyde



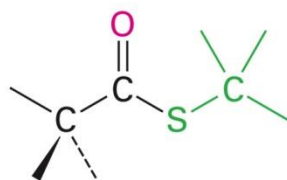
Ketone



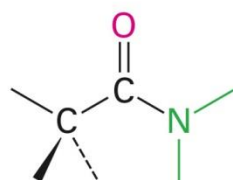
Carboxylic acid



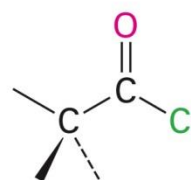
Ester



Thioester



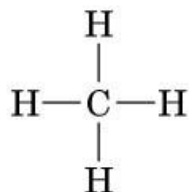
Amide



Acid chloride

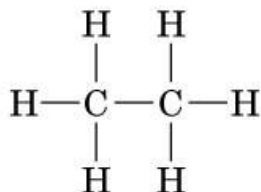
2.2 Alkanes and Alkyl Groups: Isomers

- Alkanes: Compounds with C-C single bonds and C-H bonds only (no functional groups)
- Connecting carbons can lead to large or small molecules
- The formula for an alkane with no rings in it must be C_nH_{2n+2} where the number of C's is n
- Alkanes are **saturated with hydrogen** (no more can be added)
- They are also called **aliphatic compounds**

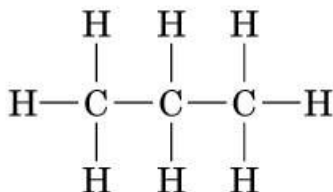


Methane

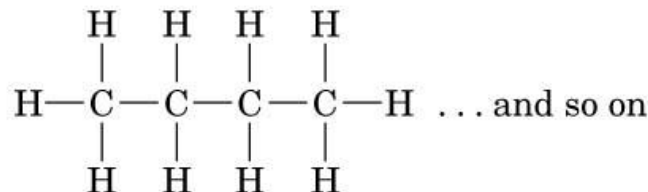
© Thomson - Brooks Cole



Ethane



Propane



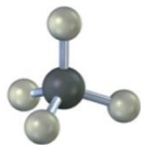
Butane

Alkane Isomers

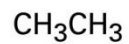
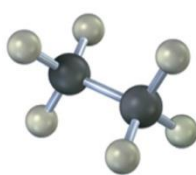
- CH_4 = methane, C_2H_6 = ethane, C_3H_8 = propane
- The molecular formula of an alkane with more than three carbons can give more than one structure
 - C_4 (butane) = butane and isobutane
 - C_5 (pentane) = pentane, **2-methylbutane**, and **2,2-dimethylpropane**
- Alkanes with C's connected to no more than 2 other C's are **straight-chain** or **normal alkanes**
- Alkanes with one or more C's connected to 3 or 4 C's are **branched-chain alkanes**
- Isomers that **differ in how their atoms are arranged** in chains are called **constitutional isomers**

Table 2.2**Names of Straight-Chain Alkanes**

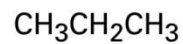
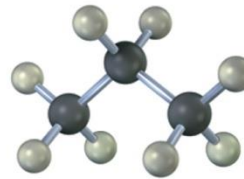
Number of carbons (n)	Name	Formula (C_nH_{2n+2})	Number of carbons (n)	Name	Formula (C_nH_{2n+2})
1	Methane	CH ₄	9	Nonane	C ₉ H ₂₀
2	Ethane	C ₂ H ₆	10	Decane	C ₁₀ H ₂₂
3	Propane	C ₃ H ₈	11	Undecane	C ₁₁ H ₂₄
4	Butane	C ₄ H ₁₀	12	Dodecane	C ₁₂ H ₂₆
5	Pentane	C ₅ H ₁₂	13	Tridecane	C ₁₃ H ₂₈
6	Hexane	C ₆ H ₁₄	20	Icosane	C ₂₀ H ₄₂
7	Heptane	C ₇ H ₁₆	30	Triacontane	C ₃₀ H ₆₂
8	Octane	C ₈ H ₁₈			



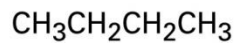
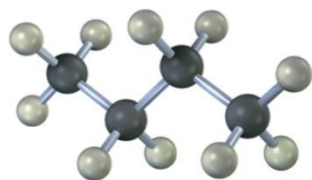
Methane, CH₄



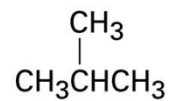
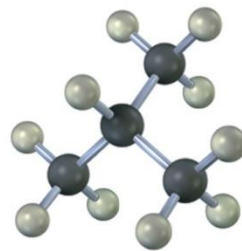
Ethane, C₂H₆



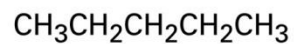
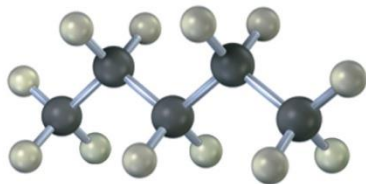
Propane, C₃H₈



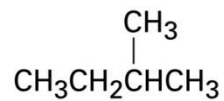
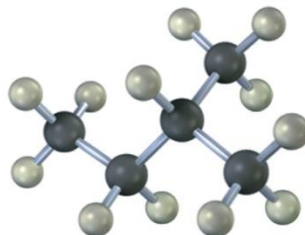
Butane, C₄H₁₀



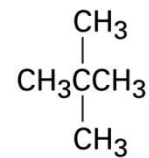
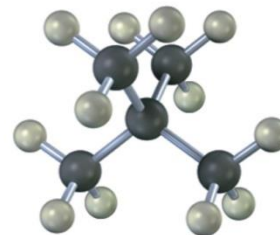
**Isobutane, C₄H₁₀
(2-methylpropane)**



Pentane, C₅H₁₂



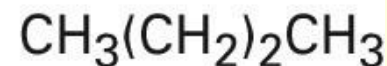
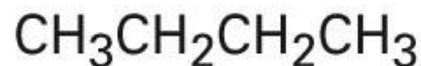
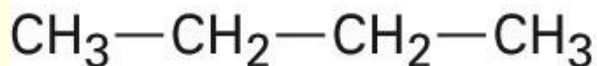
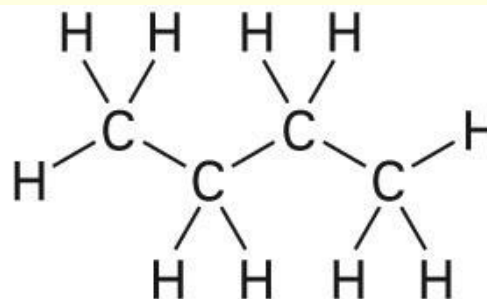
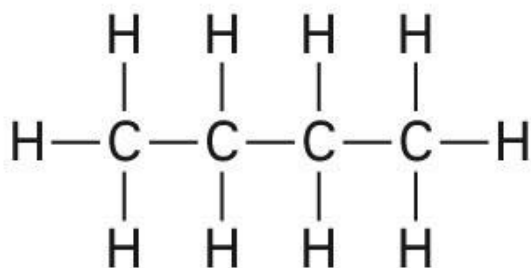
2-Methylbutane, C₅H₁₂



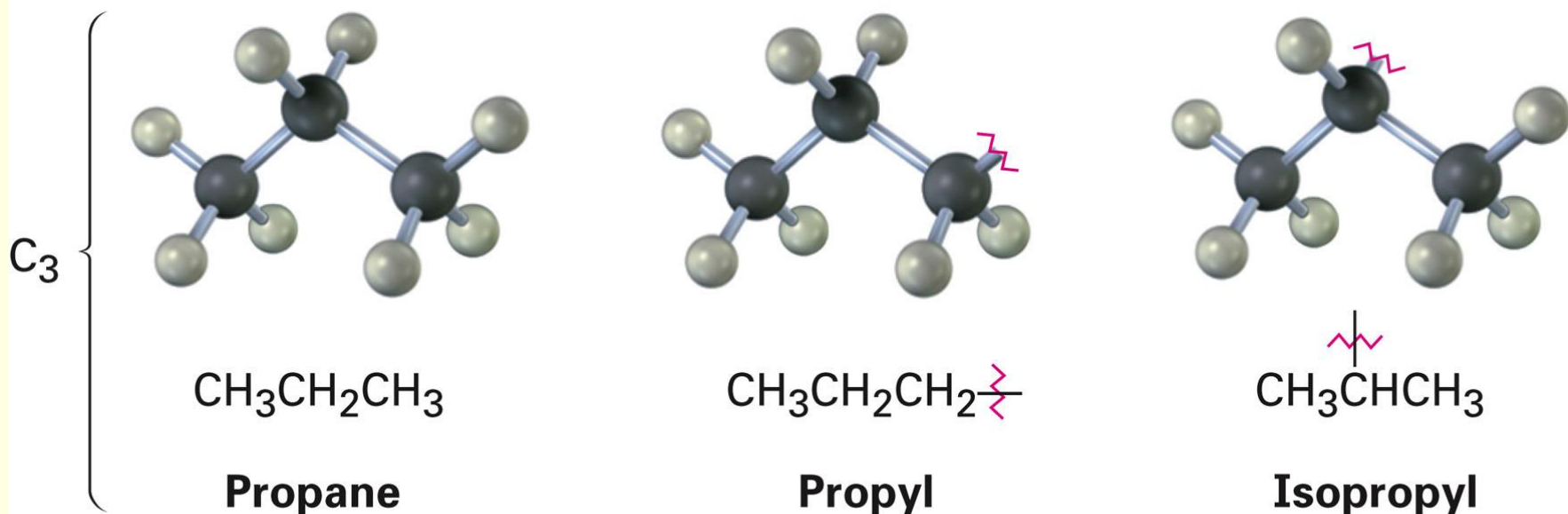
2,2-Dimethylpropane, C₅H₁₂

Condensed Structures of Alkanes

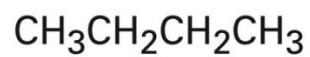
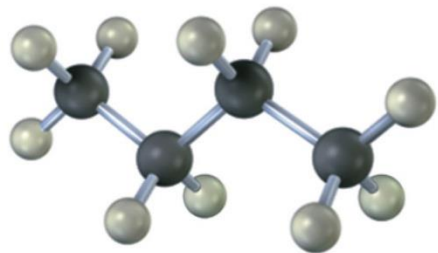
- We can represent an alkane in a brief form or in many types of extended form
- A **condensed structure does not show bonds** but lists atoms, such as
 - $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$ (butane)
 - $\text{CH}_3(\text{CH}_2)_2\text{CH}_3$ (butane)



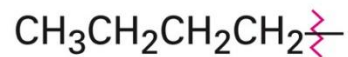
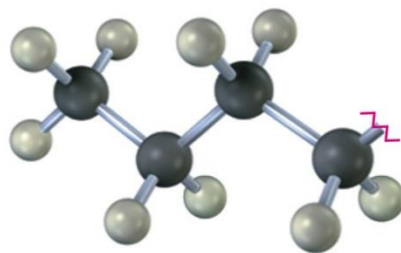
- **Alkyl group** – remove one H from an alkane (a part of a structure)
- General abbreviation “R” (for Radical, an incomplete species or the “rest” of the molecule)
- Name: replace *-ane* ending of alkane with *-yl* ending
 - CH_3 is “methyl” (from methane)
 - CH_2CH_3 is “ethyl” from ethane



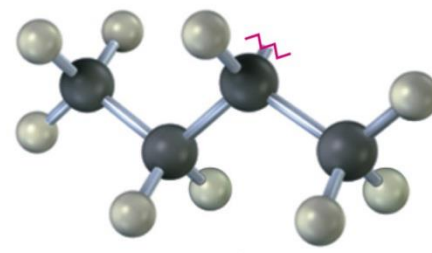
C₄



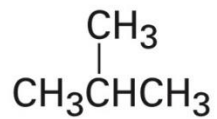
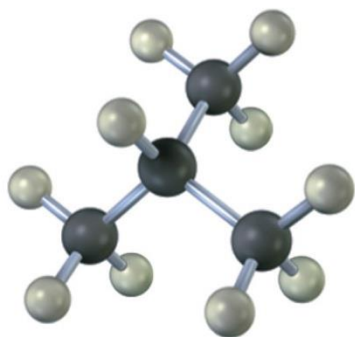
Butane



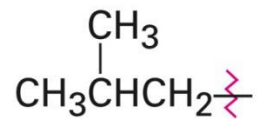
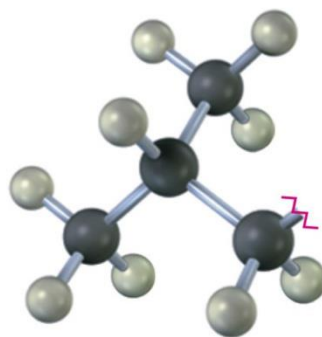
Butyl



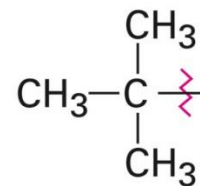
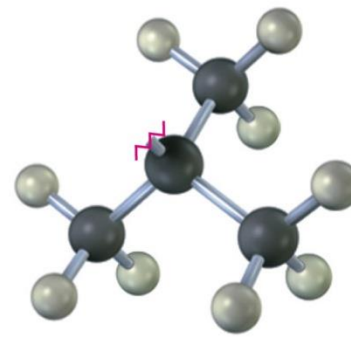
***sec*-Butyl**



Isobutane



Isobutyl



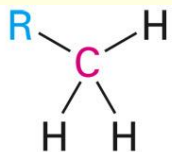
***tert*-Butyl**

Table 2.3**Some Straight-Chain Alkyl Groups**

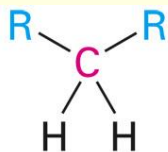
Alkane	Name	Alkyl group	Name (abbreviation)
CH_4	Methane	$-\text{CH}_3$	Methyl (Me)
CH_3CH_3	Ethane	$-\text{CH}_2\text{CH}_3$	Ethyl (Et)
$\text{CH}_3\text{CH}_2\text{CH}_3$	Propane	$-\text{CH}_2\text{CH}_2\text{CH}_3$	Propyl (Pr)
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$	Butane	$-\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	Butyl (Bu)
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	Pentane	$-\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	Pentyl, or amyl

Types of Alkyl groups

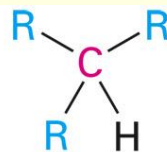
- Classified by the connection site
 - a carbon at the end of a chain (primary alkyl group)
 - a carbon in the middle of a chain (secondary alkyl group)
 - a carbon with three carbons attached to it (tertiary alkyl group)



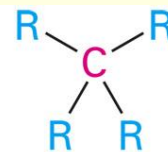
Primary carbon (1°)
is bonded to one
other carbon.



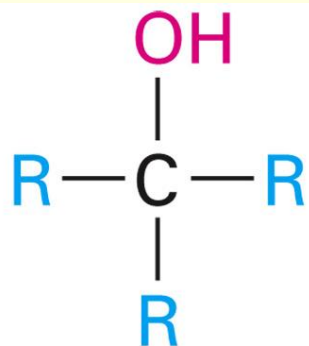
Secondary carbon (2°)
is bonded to two
other carbons.



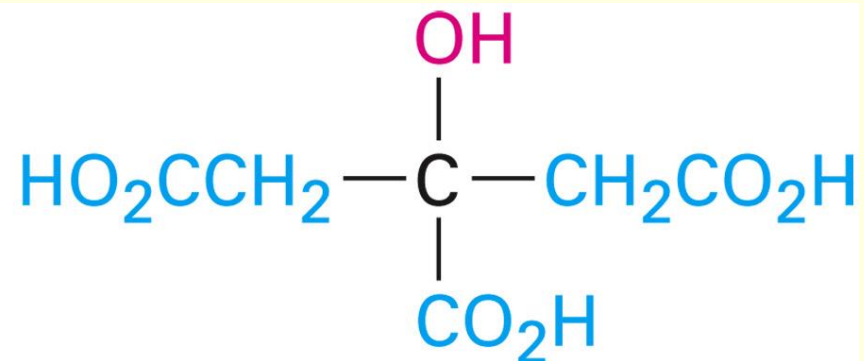
Tertiary carbon (3°)
is bonded to three
other carbons.



Quaternary carbon (4°)
is bonded to four
other carbons.



**General class of tertiary
alcohols, R_3COH**



**Citric acid—a specific
tertiary alcohol**

Worked Example 2.1

Drawing Isomeric Structures

Propose structures for two isomers with the formula $\text{C}_2\text{H}_6\text{O}$.

Strategy

We know that carbon forms four bonds, oxygen forms two, and hydrogen forms one. Put the pieces together by trial and error, along with intuition.

Solution

There are two possibilities:

