Organic chemistry

Introduction to Organic chemistry

Organic chemistry : is a is the branch of chemistry that deals with carbon and its compounds. It is fundamental to biology and medicine. Carbon is known to form unlimited number of compounds. Carbon atoms can form chains, they have branches and crosslinks. or rings of all sizes;
Organic chemicals were used in ancient times by Romans and Egyptians as dyes, medicines and poisons from natural sources, but the chemical composition of the substances was unknown . In the 16th century organic compounds were isolated from nature in the pure state and analytical methods were developed for determination of elemental composition.

Alkane

A hydrocarbon is a compound composed of only carbon and hydrogen. Figure 1 shows the four classes of hydrocarbons, along with the characteristic type of bonding between carbon atoms in each class.

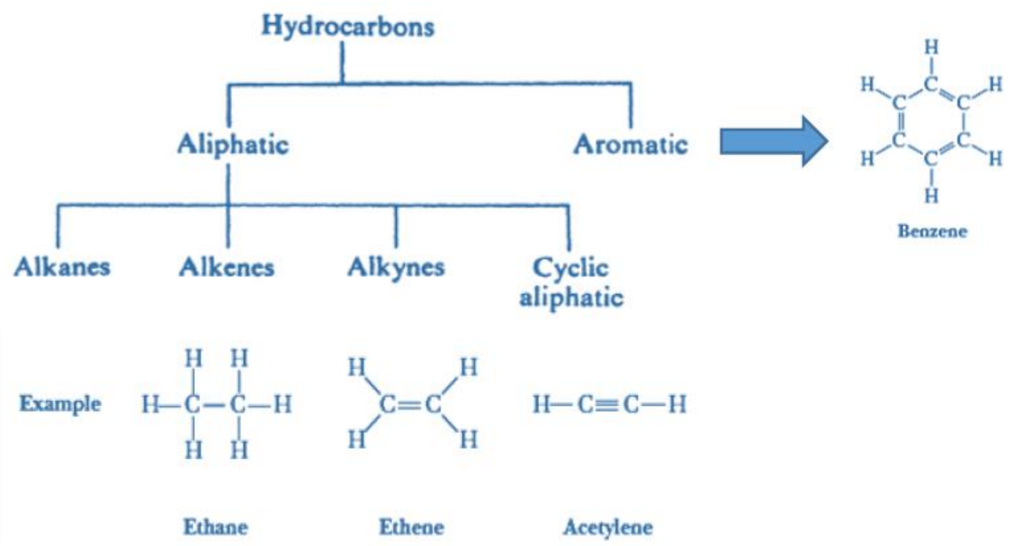


Figure 1

Alkanes are the simplest type of organic compounds and member of a larger class of organic compounds called saturated hydrocarbons that contains **only carbon–carbon single bonds**. Alkanes have the general molecular formula **CnH2n+2**. we can determine the number of hydrogens in the molecule and its molecular formula. For example, decane, with ten carbon atoms, must have (2 ×10)+ 2= 22 hydrogen atoms and a molecular formula of $C_{10}H_{22}$.

Nomenclature of Alkanes and the IUPAC System

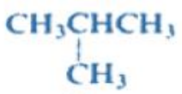
1. The rules of the IUPAC system for naming alkanes follow

The name for an alkane with an un branched chain of carbon atoms consists of a prefix showing the number of carbon atoms in the chain and the ending -**ane**. The simplest member of Alkane family is methane

Molecular Formula	Structural formula	Name
CH_4	CH_4	Methane
C_2H_6	CH3 – CH_3	Ethane
C_3H_8	CH3 – CH_2–CH3	Propane
C_4H_{10}	CH3 – CH_2–CH2–CH_3	Butane
C_5H_{12}	CH3 – CH_2–CH2–CH_2–CH_3	Pentane
C_6H_{14}	CH3 – CH_2–CH2–CH_2–CH_2–CH_3	Hexane
C_7H_{16}	CH3 – CH_2–CH2–CH_2–CH_2–CH_2–CH_3	Heptane
C_8H_{18}	CH3 – CH_2–CH2–CH_2–CH_2–CH_2–CH_2–CH_3	octane

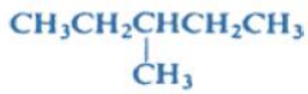
2. For branched-chain alkanes, select the longest chain of carbon atoms as the parent chain; its name becomes the root name. If there is one substituent, number the parent chain from the end that gives the substituent the lower number.

3. Give each substituent on the parent chain a name and a number. The number shows the carbon atom of the parent chain to which the substituent is bonded. Use a hyphen (-) to connect the number to the name.



I
Methylpropane
(Isobutane)

II
2-Methylpentane



III
3-Methylpentane

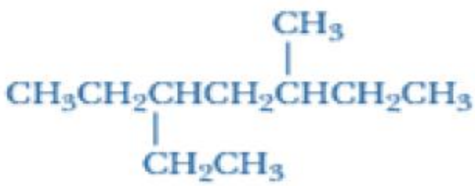
A substituent group derived from an alkane by the removal of a hydrogen atom is called an alkyl group; it is commonly represented by the symbol R -. We name alkyl groups by dropping the -ane from the name of the parent alkane and adding the suffix-yl. The substituent derived from methane, for example, is methyl

Group	Name
CH_3-	Methyl
CH_3-CH_2-	Ethyl
$CH_3-CH_2-CH_2-$	Propyl
$CH_3-CH(CH_3)-$	iso-propyl
$CH_3-CH_2-CH_2-CH_2$	butyl
$CH_3-CH(CH_3)-CH_2-$	iso-butyl
$CH_3-C(CH_3)_2-$	tert - butyl

4. If there are two or more identical substituents, number the parent chain from the end that gives the lower number to the substituent encountered first. The number of times the substituent occurs is indicated by the prefix di-, tri-, tetra-, and so on. A comma is used to separate position numbers.

2,4-Dimethylhexane **(not 3,5-dimethylhexane)**

5. If there are two or more different substituents, list them in alphabetical order and number the chain from the end that gives the lower number to the substituent encountered first

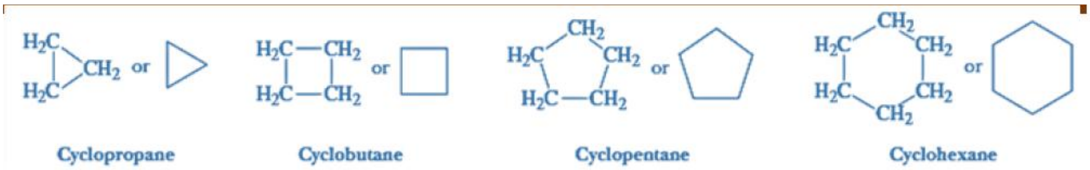


3-Ethyl-5-methylheptane (not 3-methyl-5-ethylheptane)

F-	Foloro
Br-	Bromo
I-	Iodo
NO_2 -	Nitro

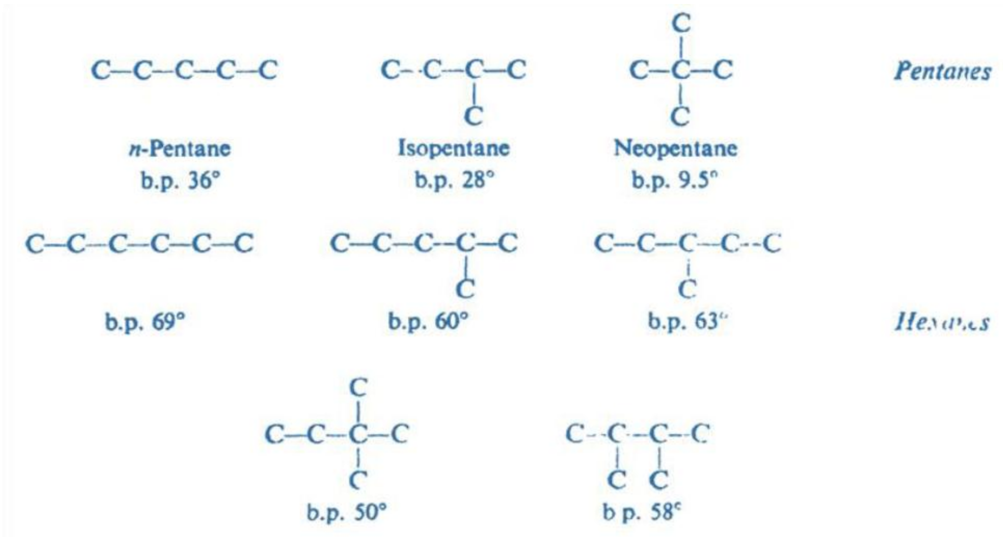
Cvclo ALkanes

A hydrocarbon that contains carbon atoms joined to form a ring is called a cyclic hydrocarbon. When all carbons of the ring are saturated, the hydrocarbon is called a cycloalkane



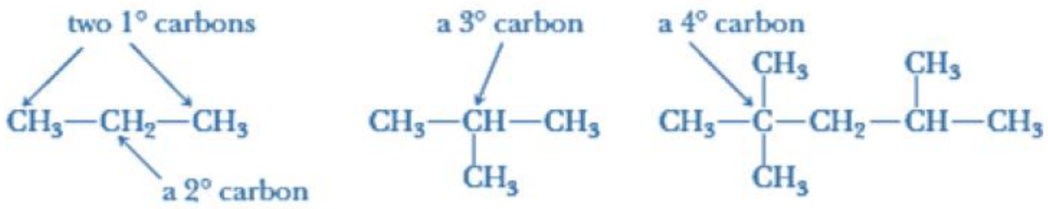
Isomers: These are different compounds that have the same molecular formula. Isomers may be structural isomers or geometrical isomersor others

Example of structural isomers



Classification of Carbon and Hydrogen Atoms

We classify a carbon atom as primary (1°), secondary (2°), tertiary (3°), or quaternary(4°)depending on the number of carbon atoms bonded to it. A carbon bonded to one carbon atom is a primary carbon; a carbon bonded to two carbon atoms is a secondary carbon for example

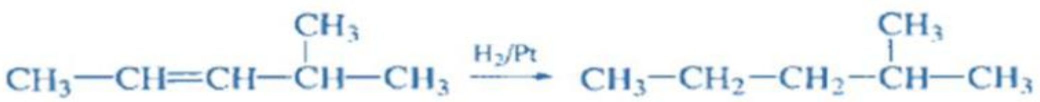


Propane 2-Methylpropane 2,2,4-Trimethylpentane

hydrogen's are also classified as primary, secondary, or tertiary depending on the type of carbon to which each is bonded. Those bonded to a primary carbon are as primary hydrogen's, those bonded to a secondary carbon are classified secondary hydrogen's, and those bonded to a tertiary carbon are tertiary hydrogen.

Preparation of Alkane

1. Hydrogenation of Alkene



2. Reduction with Alkyl Halide

A) Hydrolysis with Grignard reagent.

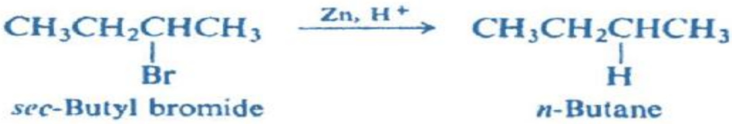
$$RX + Mg \longrightarrow RMgX \xrightarrow{H_2O} RH$$

Example:

b) Reduction with Metal and Acid

$$RX + Zn + H^+ \longrightarrow RH + Zn^{++} + X^-$$

Example:



Reaction of Alkanes

They are quite unreactive toward most reagents, a behavior consistent with the fact that they are nonpolar compounds containing only strong sigma bonds.

A) Reaction with Halogens: Halogenation

If we mix methane with chlorine or bromine in the dark at room temperature, nothing happens. If, however, we heat the mixture to 100°C or higher or expose it to light, a reaction begins at once. The products of the reaction between methane and chlorine are chloromethane and hydrogen chloride. What occurs is a substitution reaction—in this case, the substitution of chlorine for hydrogen in methane.

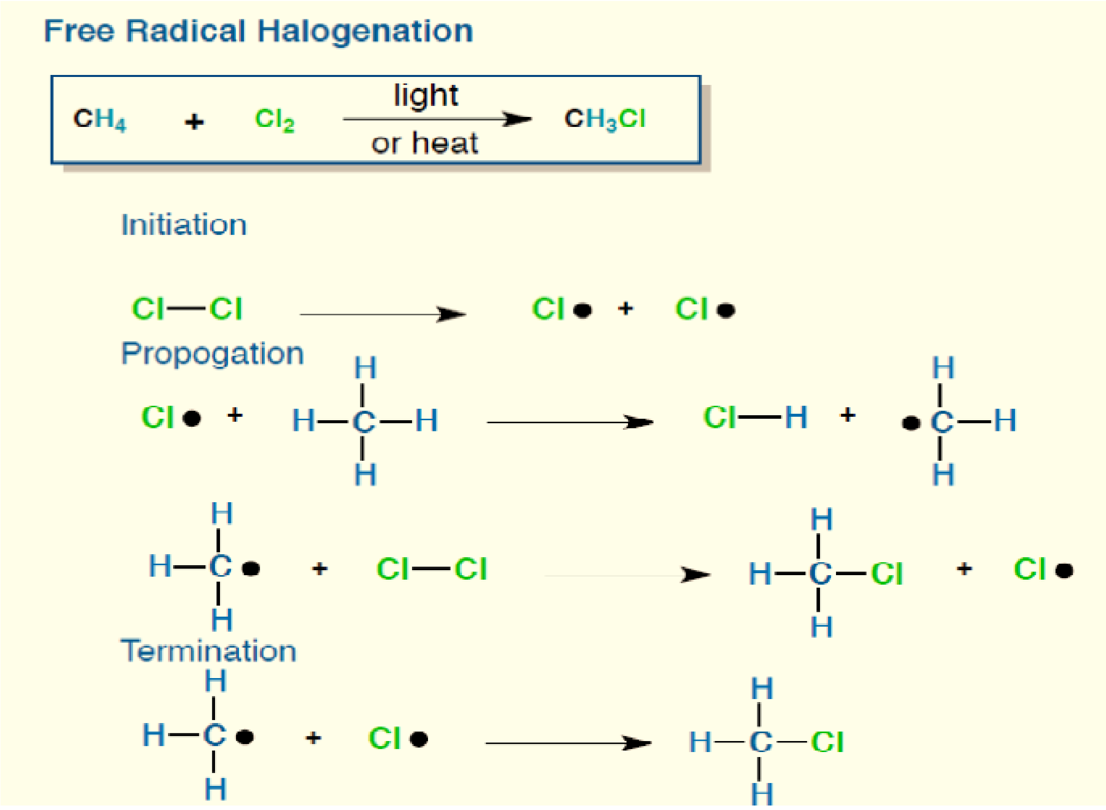
$$\underset{\text{Methane}}{CH_4} \xrightarrow{Cl_2} \underset{\text{Methyl chloride}}{HCl + CH_3Cl} \xrightarrow{Cl_2} \underset{\text{Methylene chloride}}{HCl + CH_2Cl_2} \xrightarrow{Cl_2} \underset{\text{Chloroform}}{HCl + CHCl_3} \xrightarrow{Cl_2} \underset{\text{Carbon tetrachloride}}{HCl + CCl_4}$$

Heat or light required

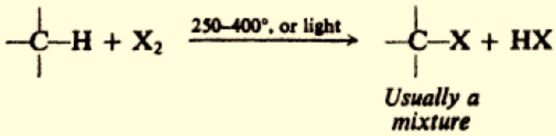
$$\underset{\text{Methane}}{CH_4} \xrightarrow{Br_2} \underset{\text{Methyl bromide}}{\overset{HBr + }{CH_3Br}} \xrightarrow{Br_2} \underset{\text{Methylene bromide}}{\overset{HBr +}{CH_2Br_2}} \xrightarrow{Br_2} \underset{\text{Bromoform}}{\overset{HBr +}{CHBr_3}} \xrightarrow{Br_2} \underset{\text{Carbon tetrabromide}}{\overset{HBr +}{CBr_4}}$$

Heat or light required

Mechanism:



In General:



Reactivity X_2: $Cl_2 > Br_2$

H: $3° > 2° > 1° > CH_3—H$

Depending upon which hydrogen is replaced ,Any of a number of isomeric product can be formed from a single of alkane

$$\underset{\text{Ethane}}{CH_3CH_3} \xrightarrow[\text{light, } 25^\circ]{Cl_2} \underset{\substack{\text{b.p. } 13^\circ \\ \text{Chloroethane} \\ \text{Ethyl chloride}}}{CH_3CH_2{-}Cl}$$

$$\underset{\text{Propane}}{CH_3CH_2CH_3} \xrightarrow[\text{light, } 25^\circ]{Cl_2} \underset{\substack{\text{b.p. } 47^\circ \\ \text{1-Chloropropane} \\ n\text{-Propyl chloride} \\ 45\%}}{CH_3CH_2CH_2{-}Cl} \quad \text{and} \quad \underset{\substack{| \\ Cl \\ \text{b.p. } 36^\circ \\ \text{2-Chloropropane} \\ \text{Isopropyl chloride} \\ 55\%}}{CH_3CHCH_3}$$

$$\underset{n\text{-Butane}}{CH_3CH_2CH_2CH_3} \xrightarrow[\text{light, } 25^\circ]{Cl_2} \underset{\substack{\text{b.p. } 78.5^\circ \\ \text{1-Chlorobutane} \\ n\text{-Butyl chloride} \\ 28\%}}{CH_3CH_2CH_2CH_2{-}Cl} \quad \text{and} \quad \underset{\substack{| \\ Cl \\ \text{b.p. } 68^\circ \\ \text{2-Chlorobutane} \\ sec\text{-Butyl chloride}}}{CH_3CH_2CHCH_3}$$

Bromination gives the corresponding bromides but in different proportions:

$$\underset{\text{Ethane}}{CH_3CH_3} \xrightarrow[\text{light, } 127^\circ]{Br_2} CH_3CH_2Br$$

$$\underset{\text{Propane}}{CH_3CH_2CH_3} \xrightarrow[\text{light, } 127^\circ]{Br_2} \underset{3\%}{CH_3CH_2CH_2Br} \quad \text{and} \quad \underset{\substack{| \\ Br \\ 97\%}}{CH_3CHCH_3}$$

$$\underset{n\text{-Butane}}{CH_3CH_2CH_2CH_3} \xrightarrow[\text{light, } 127^\circ]{Br_2} \underset{2\%}{CH_3CH_2CH_2CH_2Br} \quad \text{and} \quad \underset{\substack{| \\ Br \\ 98\%}}{CH_3CH_2CHCH_3}$$

A. Reaction with Oxygen: Combustion

Under certain conditions, however, alkanes and cycloalkanes do react, with oxygen, O_2 . By far their most important reaction with oxygen is oxidation (combustion) to form carbon dioxide and water. The oxidation of saturated hydrocarbons is the basis for their use as energy sources for heat when balancing equations for combustion reactions of hydrocarbons, first balance the number of carbons, next balance the number of hydrogens, then balance the number of oxygens. If the equation is still not balanced, consider doubling all coefficients on each side of the equation arrow

$$\underset{\text{Methane}}{CH_4} + 2O_2 \longrightarrow CO_2 + 2H_2O \quad \Delta H^\circ = -886\ kJ/mol(-212\ kcal/mol)$$

$$\underset{\text{Propane}}{CH_3CH_2CH_3} + 5O_2 \longrightarrow 3CO_2 + 4H_2O \quad \Delta H^\circ = -2{,}220\ kJ/mol(-530\ kcal/mol)$$

Physical Properties of Alkanes:

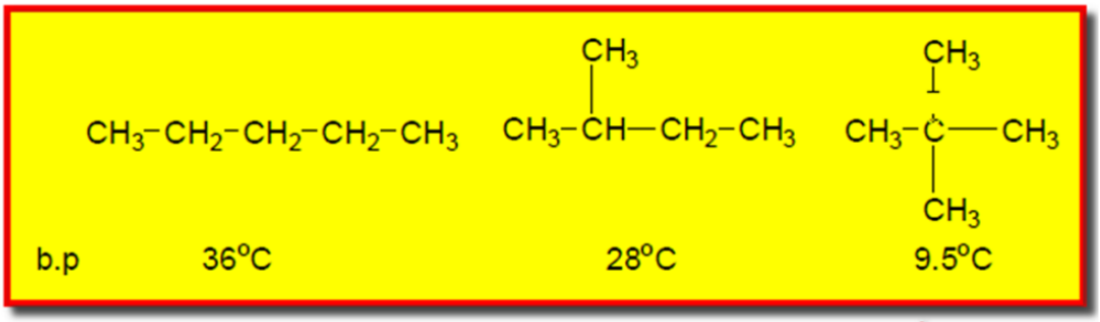
The first four n-alkanes are gases, but, as a result of the rise in boiling point and melting point with increasing chain length, the next 13 (C5-C17) are liquids, and those- containing 18 carbons or more are solids physical constants for a number of the n-alkanes., the boiling points and melting points rise as the number of carbons increases .The processes of boiling and melting require overcoming the intermolecular forces of a liquid and a solid; the boiling points and melting points rise because these intermolecular forces increase as the molecules get larger.

There are somewhat smaller differences among the boiling points of alkanes that have the same carbon number but different structures. the boiling points of the isomeric butanes, pentanes, and hexanes are given. We see that in every case a branched-chain isomer has a lower boiling point than a straight-chain isomer, and further, that the more numerous the branches, the lower the boiling point.

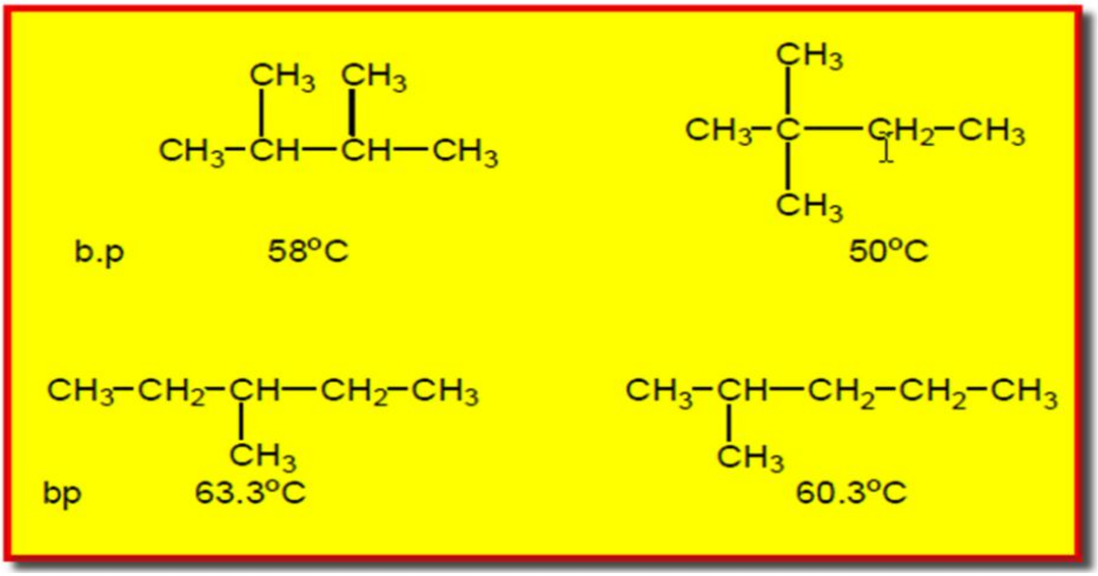
The boiling point increases steadily with increasing molecular weight regardless of the structural composition of the molecule

	CH_4	$CH_3{-}CH_3$	$CH_3{-}CH_2{-}CH_3$
b.p	-162°C	-88°C	-42°C

A- The boiling point decreases by increasing the branching on the chain, as these branches work to separate the particles from each other, thereby reducing Vander Val forces. For example, the boiling points of the molecular formula C5H12 are:



B- The boiling point increases with the symmetry of the compound molecule due to the uniformity of its molecule shape, for example: C6H14 molecular formula



C- The boiling point of cycloalkanes is higher than the boiling point of alkanes

	n-Hexane	Cyclohexane
b.p	69°C	81°C

The increase in melting point is not quite so regular, since the intermolecular forces in a crystal depend not only upon the size of the molecules but also upon how well they fit into a crystal lattice.

In agreement with the rule of thumb, "like dissolves like," the alkanes are soluble in non-polar solvents such as benzene, ether, and chloroform, and are insoluble in water and other highly polar solvents. Considered themselves as vents, the liquid alkanes dissolve compounds of low polarity and do not dissolve compounds of high polarity.

Properties

Least Polar **Most Polar**

$$\left\{\begin{matrix} \textit{alkane} \\ \textit{alkene} \\ \textit{alkyne} \end{matrix}\right\} < \text{ether} < \left\{\begin{matrix} \textit{aldehyde} \\ \textit{ketone} \end{matrix}\right\} < \text{ester} < \text{amine} < \text{amide} < \left\{\begin{matrix} \textit{alcohol} \\ \textit{phenol} \end{matrix}\right\} < \text{carboxylic acid}$$

Lowest b.p. **Highest b.p.**

Lowest water solubility **Highest water solubility**

The density increases with size of the alkanes, but tends to level off at about0.8; thus all alkanes are less dense than water. It is not surprising that nearly all organic compounds are less dense than water since, like the alkanes, they consist chiefly of carbon and hydrogen. In general, to be denser than water a compound must contain a heavy atom like bromine or iodine, or several atoms like chlorine.