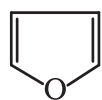
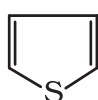


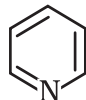
Heterocyclic aromatic compounds



Furan



Thiophene



Pyridine

Organic compounds can also be classified on the basis of functional groups, into *families* or *homologous series*.

Functional Group

The functional group may be defined as an atom or group of atoms joined in a specific manner which is responsible for the characteristic chemical properties of the organic compounds. The examples are hydroxyl group (–OH), aldehyde group (–CHO) and carboxylic acid group (–COOH) etc.

Homologous Series

A group or a series of organic compounds each containing a characteristic functional group forms a homologous series and the members of the series are called *homologues*. The members of a homologous series can be represented by general molecular formula and the successive members differ from each other in molecular formula by a $-\text{CH}_2$ unit. There are a number of homologous series of organic compounds. Some of these are alkanes, alkenes, alkynes, haloalkanes, alkanols, alkanals, alkanones, alkanolic acids, amines etc.

12.5 NOMENCLATURE OF ORGANIC COMPOUNDS

Organic chemistry deals with millions of compounds. In order to clearly identify them, a systematic method of naming has been developed and is known as the **IUPAC (International Union of Pure and Applied Chemistry)** system of nomenclature. In this systematic nomenclature, the names are correlated with the structure such that the reader or listener can deduce the structure from the name.

Before the IUPAC system of nomenclature, however, organic compounds were assigned names based on their origin or certain properties. For instance, citric acid is named so because it is found in citrus fruits and the

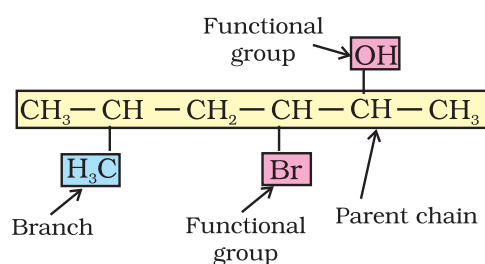
acid found in red ant is named formic acid since the Latin word for ant is *formica*. These names are traditional and are considered as *trivial* or *common names*. Some common names are followed even today. For example, Buckminsterfullerene is a common name given to the newly discovered C_{60} cluster (a form of carbon) noting its structural similarity to the geodesic domes popularised by the famous architect R. Buckminster Fuller. Common names are useful and in many cases indispensable, particularly when the alternative systematic names are lengthy and complicated. Common names of some organic compounds are given in Table 12.1.

Table 12.1 Common or Trivial Names of Some Organic Compounds

Compound	Common name
CH_4	Methane
$\text{H}_3\text{CCH}_2\text{CH}_2\text{CH}_3$	<i>n</i> -Butane
$(\text{H}_3\text{C})_2\text{CHCH}_3$	Isobutane
$(\text{H}_3\text{C})_4\text{C}$	Neopentane
$\text{H}_3\text{CCH}_2\text{CH}_2\text{OH}$	<i>n</i> -Propyl alcohol
HCHO	Formaldehyde
$(\text{H}_3\text{C})_2\text{CO}$	Acetone
CHCl_3	Chloroform
CH_3COOH	Acetic acid
C_6H_6	Benzene
$\text{C}_6\text{H}_5\text{OCH}_3$	Anisole
$\text{C}_6\text{H}_5\text{NH}_2$	Aniline
$\text{C}_6\text{H}_5\text{COCH}_3$	Acetophenone
$\text{CH}_3\text{OCH}_2\text{CH}_3$	Ethyl methyl ether

12.5.1 The IUPAC System of Nomenclature

A systematic name of an organic compound is generally derived by identifying the parent hydrocarbon and the functional group(s) attached to it. See the example given below.



By further using *prefixes* and *suffixes*, the parent name can be modified to obtain the actual name. Compounds containing carbon and hydrogen only are called hydrocarbons. A hydrocarbon is termed saturated if it contains only carbon-carbon single bonds. The IUPAC name for a homologous series of such compounds is *alkane*. Paraffin (Latin: little affinity) was the earlier name given to these compounds. Unsaturated hydrocarbons are those, which contain at least one carbon-carbon double or triple bond.

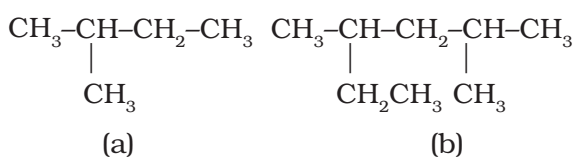
12.5.2 IUPAC Nomenclature of Alkanes

Straight chain hydrocarbons: The names of such compounds are based on their chain structure, and end with suffix '-ane' and carry a prefix indicating the number of carbon atoms present in the chain (except from CH₄ to C₄H₁₀, where the prefixes are derived from trivial names). The IUPAC names of some straight chain saturated hydrocarbons are given in Table 12.2. The alkanes in Table 12.2 differ from each other by merely the number of -CH₂ groups in the chain. They are homologues of alkane series.

Table 12.2 IUPAC Names of Some Unbranched Saturated Hydrocarbons

Name	Molecular formula	Name	Molecular formula
Methane	CH ₄	Heptane	C ₇ H ₁₆
Ethane	C ₂ H ₆	Octane	C ₈ H ₁₈
Propane	C ₃ H ₈	Nonane	C ₉ H ₂₀
Butane	C ₄ H ₁₀	Decane	C ₁₀ H ₂₂
Pentane	C ₅ H ₁₂	Icosane	C ₂₀ H ₄₂
Hexane	C ₆ H ₁₄	triacontane	C ₃₀ H ₆₂

Branched chain hydrocarbons: In a branched chain compound small chains of carbon atoms are attached at one or more carbon atoms of the parent chain. The small carbon chains (branches) are called alkyl groups. For example:

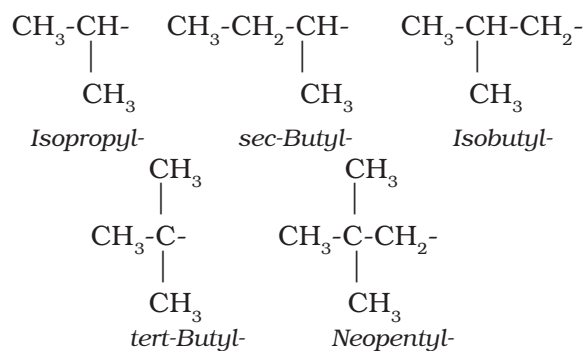


In order to name such compounds, the names of alkyl groups are prefixed to the name of parent alkane. An alkyl group is derived from a saturated hydrocarbon by removing a hydrogen atom from carbon. Thus, CH₄ becomes -CH₃ and is called *methyl group*. An alkyl group is named by substituting 'yl' for 'ane' in the corresponding alkane. Some alkyl groups are listed in Table 12.3.

Table 12.3 Some Alkyl Groups

Alkane		Alkyl group	
Molecular formula	Name of alkane	Structural formula	Name of alkyl group
CH ₄	Methane	-CH ₃	Methyl
C ₂ H ₆	Ethane	-CH ₂ CH ₃	Ethyl
C ₃ H ₈	Propane	-CH ₂ CH ₂ CH ₃	Propyl
C ₄ H ₁₀	Butane	-CH ₂ CH ₂ CH ₂ CH ₃	Butyl
C ₁₀ H ₂₂	Decane	-CH ₂ (CH ₂) ₈ CH ₃	Decyl

Abbreviations are used for some alkyl groups. For example, methyl is abbreviated as Me, ethyl as Et, propyl as Pr and butyl as Bu. The alkyl groups can be branched also. Thus, propyl and butyl groups can have branched structures as shown below.



Common branched groups have specific trivial names. For example, the propyl groups can either be *n*-propyl group or isopropyl group. The branched butyl groups are called *sec*-butyl, *isobutyl* and *tert*-butyl group. We also encounter the structural unit, -CH₂C(CH₃)₃, which is called *neopentyl* group.

Nomenclature of branched chain alkanes: We encounter a number of branched chain alkanes. The rules for naming them are given below.

chemical reactivity in an organic molecule. Compounds having the same functional group undergo similar reactions. For example, CH_3OH , $\text{CH}_3\text{CH}_2\text{OH}$, and $(\text{CH}_3)_2\text{CHOH}$ — all having -OH functional group liberate hydrogen on reaction with sodium metal. The presence of functional groups enables systematisation of organic compounds into different classes. Examples of some functional groups with their prefixes and suffixes along with some examples of organic compounds possessing these are given in Table 12.4.

First of all, the functional group present in the molecule is identified which determines the choice of appropriate suffix. **The longest chain of carbon atoms containing the functional group is numbered in such a way that the functional group is attached at the carbon atom possessing lowest possible number in the chain.** By using the suffix as given in Table 12.4, the name of the compound is arrived at.

In the case of polyfunctional compounds, one of the functional groups is chosen as the *principal functional group* and the compound is then named on that basis. The remaining functional groups, which are subordinate functional groups, are named as substituents using the appropriate prefixes. The choice of principal functional group is made on the basis of order of preference. **The order of decreasing priority for some functional groups is:**

-COOH, -SO₃H, -COOR (R=alkyl group), COCl, -CONH₂, -CN, -HC=O, >C=O, -OH, -NH₂, >C=C<, -C≡C-

The -R, C₆H₅-, halogens (F, Cl, Br, I), -NO₂, alkoxy (-OR) etc. are always prefix substituents. Thus, a compound containing both an alcohol and a keto group is named as hydroxyalkanone since the keto group is preferred to the hydroxyl group.

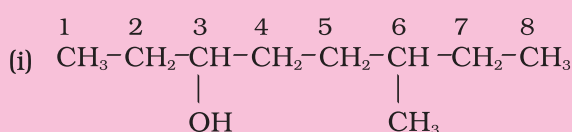
For example, $\text{HOCH}_2(\text{CH}_2)_3\text{CH}_2\text{COCH}_3$ will be named as 7-hydroxyheptan-2-one and not as 2-oxoheptan-7-ol. Similarly, $\text{BrCH}_2\text{CH}=\text{CH}_2$ is named as 3-bromoprop-1-ene and not 1-bromoprop-2-ene.

If more than one functional group of the same type are present, their number is indicated by adding di, tri, etc. before the class

suffix. In such cases the full name of the parent alkane is written before the class suffix. For example $\text{CH}_2(\text{OH})\text{CH}_2(\text{OH})$ is named as ethane-1,2-diol. However, the ending -ne of the parent alkane is dropped in the case of compounds having more than one double or triple bond; for example, $\text{CH}_2=\text{CH}-\text{CH}=\text{CH}_2$ is named as buta-1,3-diene.

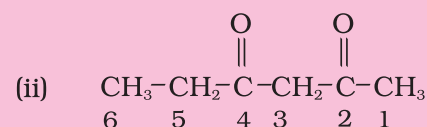
Problem 12.8

Write the IUPAC names of the compounds i-iv from their given structures.



Solution

- The functional group present is an alcohol (OH). Hence the suffix is '-ol'.
- The longest chain containing -OH has eight carbon atoms. Hence the corresponding saturated hydrocarbon is octane.
- The -OH is on carbon atom 3. In addition, a methyl group is attached at 6th carbon. Hence, the systematic name of this compound is 6-Methyloctan-3-ol.



Solution

The functional group present is ketone (>C=O), hence suffix '-one'. Presence of two keto groups is indicated by 'di', hence suffix becomes 'dione'. The two keto groups are at carbons 2 and 4. The longest chain contains 6 carbon atoms, hence, parent hydrocarbon is hexane. Thus, the systematic name is Hexane-2,4-dione.

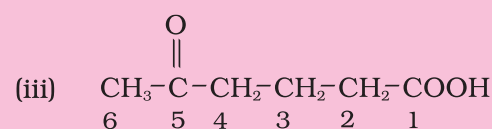

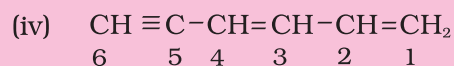


Table 12.4 Some Functional Groups and Classes of Organic Compounds

Class of compounds	Functional group structure	IUPAC group prefix	IUPAC group suffix	Example
Alkanes	-	-	-ane	Butane, $\text{CH}_3(\text{CH}_2)_2\text{CH}_3$
Alkenes	$>\text{C}=\text{C}<$	-	-ene	But-1-ene, $\text{CH}_2=\text{CHCH}_2\text{CH}_3$
Alkynes	$-\text{C}\equiv\text{C}-$	-	-yne	But-1-yne, $\text{CH}\equiv\text{CCH}_2\text{CH}_3$
Arenes	-	-	-	Benzene, 
Halides	-X (X=F, Cl, Br, I)	halo-	-	1-Bromobutane, $\text{CH}_3(\text{CH}_2)_2\text{CH}_2\text{Br}$
Alcohols	-OH	hydroxy-	-ol	Butan-2-ol, $\text{CH}_3\text{CH}_2\text{CHOHCH}_3$
Aldehydes	-CHO	formyl, or oxo	-al	Butanal, $\text{CH}_3(\text{CH}_2)_2\text{CHO}$
Ketones	$>\text{C}=\text{O}$	oxo-	-one	Butan-2-one, $\text{CH}_3\text{CH}_2\text{COCH}_3$
Nitriles	$-\text{C}\equiv\text{N}$	cyano	nitrile	Pentanenitrile, $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CN}$
Ethers	-R-O-R-	alkoxy-	-	Ethoxyethane, $\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3$
Carboxylic acids	-COOH	carboxy	-oic acid	Butanoic acid, $\text{CH}_3(\text{CH}_2)_2\text{CO}_2\text{H}$
Carboxylate ions	$-\text{COO}^-$	-	-oate	Sodium butanoate, $\text{CH}_3(\text{CH}_2)_2\text{CO}_2^- \text{Na}^+$
Esters	-COOR	alkoxycarbonyl	-oate	Methyl propanoate, $\text{CH}_3\text{CH}_2\text{COOCH}_3$
Acyl halides	-COX (X=F, Cl, Br, I)	halocarbonyl	-oyl halide	Butanoyl chloride, $\text{CH}_3(\text{CH}_2)_2\text{COCl}$
Amines	$-\text{NH}_2$, $>\text{NH}$, $>\text{N}-$	amino-	-amine	Butan-2-amine, $\text{CH}_3\text{CHNH}_2\text{CH}_2\text{CH}_3$
Amides	$-\text{CONH}_2$, $-\text{CONHR}$, $-\text{CONR}_2$	-carbamoyl	-amide	Butanamide, $\text{CH}_3(\text{CH}_2)_2\text{CONH}_2$
Nitro compounds	$-\text{NO}_2$	nitro	-	1-Nitrobutane, $\text{CH}_3(\text{CH}_2)_3\text{NO}_2$
Sulphonic acids	$-\text{SO}_3\text{H}$	sulpho	sulphonic acid	Methylsulphonic acid $\text{CH}_3\text{SO}_3\text{H}$

Solution

Here, two functional groups namely ketone and carboxylic acid are present. The principal functional group is the carboxylic acid group; hence the parent chain will be suffixed with 'oic' acid. Numbering of the chain starts from carbon of -COOH functional group. The keto group in the chain at carbon 5 is indicated by 'oxo'. The longest chain including the principal functional group has 6 carbon atoms; hence the parent hydrocarbon is hexane. The compound is, therefore, named as 5-Oxohexanoic acid.

**Solution**

The two C=C functional groups are present at carbon atoms 1 and 3, while the C≡C functional group is present at carbon 5. These groups are indicated by suffixes 'diene' and 'yne' respectively. The longest chain containing the functional groups has 6 carbon atoms; hence the parent hydrocarbon is hexane. The name of compound, therefore, is Hexa-1,3-dien-5-yne.

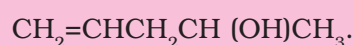
Problem 12.9

Derive the structure of (i) 2-Chlorohexane, (ii) Pent-4-en-2-ol, (iii) 3-Nitrocyclohexene, (iv) Cyclohex-2-en-1-ol, (v) 6-Hydroxyheptanal.

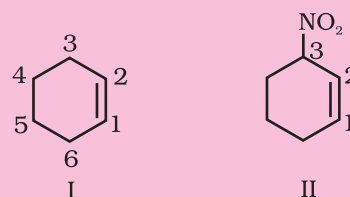
Solution

(i) 'hexane' indicates the presence of 6 carbon atoms in the chain. The functional group chloro is present at carbon 2. Hence, the structure of the compound is $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}(\text{Cl})\text{CH}_3$.

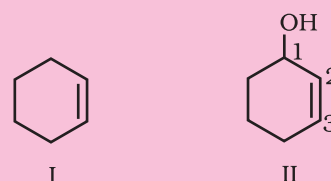
(ii) 'pent' indicates that parent hydrocarbon contains 5 carbon atoms in the chain. 'en' and 'ol' correspond to the functional groups C=C and -OH at carbon atoms 4 and 2 respectively. Thus, the structure is



(iii) Six membered ring containing a carbon-carbon double bond is implied by cyclohexene, which is numbered as shown in (I). The prefix 3-nitro means that a nitro group is present on C-3. Thus, complete structural formula of the compound is (II). Double bond is suffixed functional group whereas NO_2 is prefixed functional group therefore double bond gets preference over $-\text{NO}_2$ group:



(iv) '1-ol' means that a -OH group is present at C-1. OH is suffixed functional group and gets preference over C=C bond. Thus the structure is as shown in (II):



(v) 'heptanal' indicates the compound to be an aldehyde containing 7 carbon atoms in the parent chain. The '6-hydroxy' indicates that -OH group is present at carbon 6. Thus, the structural formula of the compound is: $\text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CHO}$. Carbon atom of -CHO group is included while numbering the carbon chain.

12.5.4 Nomenclature of Substituted Benzene Compounds

For IUPAC nomenclature of substituted benzene compounds, the substituent is placed as prefix to the word *benzene* as shown in the following examples. However, common names (written in bracket below) of many substituted benzene compounds are also universally used.