# NOMENCLATURE IN ORGANIC CHEMISTRY

Contents				
1. INTRODUCTION 3				
2. HYDROC	ARBONS	3		
(i)	Alkanes	3		
	A. Unbranched Chains	3		
	B. Unbranched chains	4		
(ii)	Alkenes	5		
	A. One double bond	5		
	B. More than one double bond	5		
	C. <i>E/Z</i> Isomers in Alkenes	6		
(iii)	Alkynes	8		
(iv)	Combined Alkenes and Alkynes	8		
(v)	Cyclic Hydrocarbons	9		
3. COMPOL	INDS CONTAINING HALOGENS AND NITRO GROUPS	10		
4. COMPOL	INDS WITH FUNCTIONAL GROUPS NAMED AS SUFFIXES	12		
(i)	General Naming Scheme	12		
	A. Choosing the Principal Chain	13		
	B. Naming the Principal Chain	13		
	C. Numbering the Principal Chain	13		
(ii)	Naming Various Classes of Organic Compounds	14		
	A. Ethers and Thioethers	14		
	B. Alcohols and Thiols	14		
	C. Acids, Salts of Acids and Acid Anhydrides	15		
	D. Esters	17		
	E. Acid Halides	18		
	F. Amides	18		
	G. Nitriles	19		
	H. Aldehydes	19		
	I. Ketones	21		
	J. Amines and Ammonium Salts	22		
5. AROMAT	IC COMPOUNDS	23		
(i)	General Notes	23		
(ii)	Aromatic Hydrocarbons	23		
(iii)	Substituted Aromatic Hydrocarbons	24		

А.	Halogen and Nitro- Substituted Aromatics	24
В.	Carboxylic Acids and Derivatives	24
C.	Phenols and Thiophenols	25
D.	Aldehydes and Ketones	26
E.	Sulfonic acids and Sulfonic Acid Derivatives	27
F.	Aromatic Amines	28
G.	Diazonium Salts	29
RADICOFUN	CTIONAL NAMING	29
A.	Alkyl Halides	29
В.	Alcohols	29
C.	Ketones	30
D.	Nitriles (or Cyanides)	30
E.	Grignard Reagents	30

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Revised and updated Professor L D Field

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1

# NOMENCLATURE IN ORGANIC CHEMISTRY

# 1. INTRODUCTION

It is important that organic compounds are corrrectly and unambiguously named so that there can be absolutely no confusion about what compounds are actually being reported or described. There have been many conventions for naming organic compounds - some have had limit scope or become embedded in common usage and some have persisted over time

The International Union of Pure and Applied Chemistry (I.U.P.A.C.) periodically reviews naming practice, attempting to standardise nomenclature. The following guidelines for organic nomenclature are based on the definitive rules published by I.U.P.A.C.<sup>1</sup> (the International Union of Pure and Applied Chemistry).

# 2. HYDROCARBONS

(i) The Alkanes (C<sub>n</sub>H<sub>2n+2</sub>)

## A. Unbranched Chains

The first four (n=1-4) unbranched chain saturated hydrocarbons are called methane, ethane, propane and butane. After this, there is a numerical term (of Greek origin) followed by the ending "-ane". The first twelve members are given in Table 1.

## Table 1.The names of the first 12 linear alkanes

n	Name	Molecular formula	Constitutional formula
1	methane	CH <sub>4</sub>	CH <sub>4</sub>
2	ethane	$C_2H_6$	CH <sub>3</sub> CH <sub>3</sub>
3	propane	C <sub>3</sub> H <sub>8</sub>	CH <sub>3</sub> CH <sub>2</sub> CH <sub>3</sub>
4	butane	C <sub>4</sub> H <sub>10</sub>	$CH_3CH_2CH_2CH_3$
5	pentane	$C_5H_{12}$	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>
6	hexane	$C_6H_{14}$	$CH_3CH_2CH_2CH_2CH_3$
7	heptane	C <sub>7</sub> H <sub>16</sub>	$CH_3CH_2CH_2CH_2CH_2CH_3$
8	octane	C <sub>8</sub> H <sub>18</sub>	$CH_{3}CH_{2}CH_{2}CH_{2}CH_{2}CH_{2}CH_{3}$
9	nonane	$C_9H_{20}$	$CH_{3}CH_{2}CH_{2}CH_{2}CH_{2}CH_{2}CH_{2}CH_{3}$
10	decane	$C_{10}H_{22}$	$CH_{3}CH_{2}CH_{2}CH_{2}CH_{2}CH_{2}CH_{2}CH_{2}CH_{3}$
11	undecane	C <sub>11</sub> H <sub>24</sub>	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$
12	dodecane	$C_{12}H_{26}$	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$

The group derived from one of these alkanes by removal of a terminal (end) hydrogen is called an alkyl group. The group name is found by removing "ane" from the alkane name and adding "yl".

Example: CH<sub>3</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>3</sub> butane becomes CH<sub>3</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-

**Note**: The free valence must be on the terminal carbon.

1

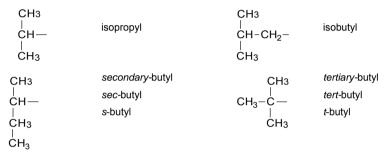
butyl

# B. Branched Chains

The following steps are taken in naming an alkane with a branched chain:

- (a) Find the longest continuous carbon chain and select the appropriate alkane name from Table 1. (Side chains are not included in the carbon count.)
- (b) Name all of the side chains (carbon chains attached to the longest chain) and list them in alphabetical order. Ignore multiplicative prefixes such as "di-" (2), "tri-" (3), "tetra-" (4) *etc.* Also ignore "sec-" and "*tert-*" but *not* "iso".
- (c) Number the longest chain so that substituents have the lowest possible numbers and insert location numbers before each of the side chain names.

Special Note: The following groups have the special names indicated:



# Examples

СН <sub>3</sub> -СН <sub>2</sub> -СН-СН <sub>2</sub> -СН <sub>3</sub>   СН <sub>3</sub>	3-methylpentane
$CH_3-CH-CH_2-CH-CH-CH_2-CH_3$ $\downarrow \qquad \downarrow \qquad \downarrow CH_3 \qquad CH_3 CH_3$	2,4,5-trimethylheptane (not 3,4,6-)
CH <sub>3</sub>	4-isopropyl-2 2-dimethylheni

 $\begin{array}{c} \mathsf{CH}_3-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{CH}-\mathsf{CH}_2-\mathsf{CH}-\mathsf{CH}_3\\ \overset{1}{\mathsf{CH}} & \overset{1}{\mathsf{CH}} \\ \mathsf{CH}_3 & \overset{1}{\mathsf{CH}}_3 \end{array}$ 

$$CH_3 - CH_2$$
 4-  
 $CH_3 - CH_2 - CH_2 - CH_2 - CH_2 - CH_2 - CH_3$  (r  
 $H_3$ 

4-isopropyl-2,2-dimethylheptane

4

4-ethyl-5-methyloctane (not 5-ethyl-4-methyloctane)

I.U.P.A.C. Nomenclature for Organic Chemistry, Sections A, B and C (combined edition), Butterworths Scientific Publications, London, 1971.

The following compounds have special names:

$$\begin{array}{c} \mathsf{CH}_3-\mathsf{CH}-\mathsf{CH}_3\\ \mathsf{CH}_3\\ \mathsf{CH}_3\\$$

Branched side chains are named by renumbering the alkyl group giving the carbon with the free valence (*i.e.* point of attachment to the main chain) the number 1 and giving substituents the appropriate number in the usual way.

#### Examples

$$\begin{array}{c} \mathsf{CH}_3\mathsf{CH}_2-\mathsf{CH}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{CH}_3\\ \mathsf{CH}_3-\mathsf{CH}-\mathsf{CH}-\mathsf{CH}_2-\mathsf{CH}-\mathsf{CH}_3\\ \mathsf{CH}_3-\mathsf{CH}-\mathsf{CH}-\mathsf{CH}_2-\mathsf{CH}-\mathsf{CH}_3\\ \mathsf{CH}_3-\mathsf{CH}_3\\ \mathsf{CH}_3\\ \mathsf{CH}_3\end{array} \qquad 1,3,4\text{-trimethylpentyl group}$$

The following example gives the name of an alkane having a branched side chain:

$$CH_{3}$$
  
 $CH_{2}-CH_{2}-CH_{2}-CH_{3}$   
 $CH_{3}-CH_{2}-CH_{2}-CH_{2}-CH_{2}-CH_{2}-CH_{2}-CH_{2}-CH_{2}$   
 $CH_{3}-CH_{2}-CH_{2}-CH_{2}-CH_{2}-CH_{2}-CH_{2}$ 

4-ethyl-6-(2-methylbutyl)undecane

~ . .

# (ii) The Alkenes (C<sub>n</sub>H<sub>2n</sub>)

## A. One double bond

- (a) Find and name the longest carbon chain **containing the double bond**.
- (b) Change the "ane" of the alkane name to "ene".
- (c) Number the carbon chain giving the double bond the lowest possible location number.
- (d) Name side chains in the usual way.

**Examples** (note position of numbers and punctuation)

CH<sub>3</sub>-CH=CH-CH<sub>3</sub>

$$CH_3 \\ CH_3 - C - CH = CH - CH_3 \\ - CH_3 \\ CH_3$$

4,4-dimethyl-2-pentene

propene 2-butene

# Special Note

 $CH_2 = CH_2$  has the special name "ethylene".

## B. More than one double bond

- (a) Find and name the longest carbon chain containing the maximum number of double bonds.
- (b) Change the "ane" of the alkane name to:
  - "adiene" 2 double bonds
  - "atriene" 3 double bonds
  - "atetraene" 4 double bonds etc.
- (c) Number the chain so as to give the double bonds the lowest possible numbers.
- (d) Name the alkyl side chains in the usual way.

#### Examples (note position of numbers and punctuation)

 $CH_2 = CH - CH = CH_2$ 

1,3-butadiene

$$CH_3-CH=CH-C=CH-CH=CH_2$$
$$I$$
$$CH_3-CH_2-CH_2-CH_2$$
$$CH_3$$

4-butyl-2-methyl-1,3,5-heptatriene

## **Special Note**

 $CH_2 = C = CH_2$  has the special name "allene".

## C. E/Z Isomers in Alkenes

In the past, the terms *cis* and *trans* have been used to differentiate the isomers; *cis* to indicate the isomer in which the substituents are on the same side of the double bond, *trans* when they are on opposite sides. This nomenclature is still used in some older texts, however, the approved nomenclature for alkene stereoisomers involves the prefixes *Z*- or *E*-.

There are two substituents attached to each of the carbon atoms which form a C=C. The carbon atoms at either end of the C=C are considered separately and at each end, the two attached substituents are ranked according to a simple set of *priority rules* (or sequence rules). The priority of the two groups attached to each carbon atom of the C=C is based initially on the atomic number of the atom at the point of attachment. For example, a chlorine

substituent would have a higher priority than a  $\mbox{CH}_3\mbox{-}$  which in turn would have a higher priority than a H-.

When the C=C is considered as a whole, if the groups with the highest priorities are on the same side of the double bond then the name of the alkene is prefixed with a Z (from the German 'zusammen' meaning 'together'). If they are on opposite sides then the prefix is E (from 'entgegen' meaning 'opposite').



#### **Priority Rules**

Each of the atoms attached directly to the C atom of a C=C is assigned a priority based on its atomic number: the higher the atomic number, the higher the priority. In terms of priority, if there is a hydrogen attached to one carbon of the C=C, it must always have the lowest priority. Groups which have an oxygen atom attached directly to the C=C (*eg.* -OH, -OCH<sub>3</sub>) have higher priority than groups which have a nitrogen atom attached directly to the C=C atom (*eg.* -NH<sub>2</sub>, -N(CH<sub>3</sub>)<sub>2</sub>) and so on.

 $-I > -Br > -CI > -OH > -NH_2 > -CH_3 > -H$ 

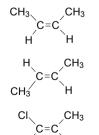
If two of the groups attached to the same carbon of a C=C begin with the same element (eg.  $-CH_3$ ,  $-CH_2CH_3$ ), then look to the next atoms away from the C=C. If the groups at this point are still the same, then move further from the C=C until the point of difference is found (there must be a point of difference somewhere). The group priority is then assigned based on the atomic numbers of the atoms at the point of difference.

So for example –CH<sub>2</sub>Cl has a higher priority than –CH<sub>2</sub>OH.

 $-CH_2Br > -CH_2Cl > -CH(CH_3)_2 > -CH_2CH_3 > -CH_3$ 

For the purposes of assigning group priorities, double bonds or multiple bonds are expanded to be an equivalent number of atoms attached by single bonds. So a  $-CH=CH_2$  group is considered as equivalent to  $-CH(-CH_2)_2$ .

#### Examples

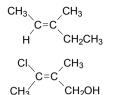


CH<sub>3</sub>

Z-2-butene

E-2-butene

Z-2-chloro-2-butene (note –Cl has higher priority than -CH<sub>3</sub>)



#### E-3-methyl-2-pentene

(note that -CH<sub>2</sub>CH<sub>3</sub> has greater priority than - CH<sub>3</sub>)

E-3-chloro-2-methyl-2-penten-1-ol

(note that –Cl has higher priority than –CH $_{\rm 3}$  and -CH $_{\rm 2}OH$  has higher priority than -CH $_{\rm 3})$ 

# (iii) The Alkynes (C<sub>n</sub>H<sub>2n-2</sub>)

These are named in identical fashion to alkenes except that "ene" in the alkene name is replaced by:

"yne"	1 triple bond
"adiyne"	2 triple bonds
"atriyne"	3 triple bonds etc.

**Example** (note position of numbers and punctuation)

 $CH_3 - C \equiv C - CH_2 - CH_3$  2-pentyne

#### Special Note

H-C=C-H has the special name "acetylene".

#### Salts of Alkynes

The salts of hydrocarbon anions are named by adding the ending "-ide" together with a location number.

### Examples

CH<sub>3</sub>−C≡C<sup>−</sup>Li<sup>+</sup>

 $H_3C - CH_2 - C \equiv C$  Na<sup>+</sup>

lithium 1-propyn-1-ide (from propyne)

sodium 1-butyn-1-ide (from 1-butyne)

#### Special Note:

н

-c≡c_		No <sup>+</sup>	$\overline{c} = c$		i
1-020	INd	INd	$C \equiv C$	INd	(

are called monosoium acetylide and disodium acetylide respectively

# (iv) Combined Alkenes and Alkynes

If a compound has double and triple bonds then the longest chain is selected so as to contain the maximum number of double **and** triple bonds and is named by replacing the "ane" of the corresponding alkane by "en(e)", "adien(e)" *etc.* followed by "yne", "diyne" *etc.* The "e" is omitted before a vowel or a "y".

The chain is numbered so as to give the lowest numbers to the double bonds, **then** triple bonds.

## **Examples** (note positions of numbers and punctuation)

$CH_2 = CH - C \equiv CH$	1-buten-3-yne
$CH_2 = CH - C \equiv C - C = CH - CH_3$	5-methyl-1,5-heptadien-3-yne
$H-C\equiv C-C\equiv C-CH=CH-CH_3$	2-hepten-4,6-diyne

Groups derived from alkenes, alkynes or combined hydrocarbons are named by dropping the final "e" and replacing it by "yl". The chain is renumbered to give the carbon with the free valence the number 1 position:

#### **Examples** (note positions of numbers and punctuation)

$H-C\equiv C-CH=CH-CH_2-$	2-penten-4-ynyl group
$H-C\equiv C-CH_2-$	2-propynyl group
$CH_3 - CH = CH - CH_2 -$	2-butenyl group
$H-C\equiv C-$	ethynyl group

### Special Note: The following have special names:

CH <sub>2</sub> =CH-	vinyl group
$CH_2 = CH - CH_2 -$	allyl group
$H-C\equiv C-CH_2-$	propargyl group

# (v) Cyclic Hydrocarbons

Compounds with hydrocarbon rings are named by the insertion of "cyclo"- before the name of the hydrocarbon corresponding to the open chain compound containing the same number of carbons.

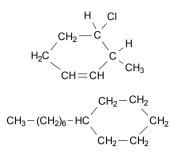
# Examples



Cyclopropane

 $\begin{array}{c} CH_2-CH_2\\ H_2C \\ CH_2-CH_2 \end{array}$ 

Cyclohexane



4-chloro-3-methyl-1-cyclohexene

1-cyclohexylheptane

(note that the carbon chain has more carbons than the ring)

# 3. COMPOUNDS CONTAINING HALOGENS AND NITRO GROUPS

The halogens (F, Cl, Br, I) and the nitro group (-NO<sub>2</sub>) are always named as prefixes in the same way as side chains on hydrocarbons. The prefixes are as follows:

Group	Prefix	
F-	fluoro	
CI-	chloro	
Br-	bromo	
I-	iodo	
NO <sub>2</sub> -	nitro	

## Examples

lodomethane  $CH_3 - I$ CH<sub>3</sub>-CH-CH<sub>3</sub> 2-chloropropane ĊI  $CH_3$ 2-bromo-2-methylpropane CH<sub>3</sub>-C-CH<sub>3</sub> Βr

$$CH_{3}-CH_{2}$$

$$CH_{3}-CH_{2}-CH-CH_{2}-CH_{2}-F$$

$$CH_{3}-CH_{2}-CH_{2}-CH_{2}-F$$

$$CH_{3}-CH_{2}-CH_{2}-CH_{2}$$

$$CH_{2}-CH_{2}-CH_{2}$$

$$CH_{2}-CH_{2}-CH_{2}$$

$$CH_{2}-CH_{2}-CH_{2}-CH_{2}$$

$$CH_{2}-$$

### Special Note: The following have special names:

 $CH_2 = CH - CH_2 - CH_2 - CI$ 

**~** · · · - . .

F <sub>3</sub> C-H	fluoroform
Cl₃C-H	chloroform
Br <sub>3</sub> C-H	bromoform
I <sub>3</sub> C-H	iodoform
CCl <sub>4</sub>	carbon tetrachloride
CBr <sub>4</sub>	carbon tetrabromide

#### COMPOUNDS WITH FUNCTIONAL GROUPS NAMED AS SUFFIXES 3

#### (i) **General Naming Scheme**

The name of every organic molecule containing a functional group whose name appears as a suffix may be thought of as made up of four parts:

Numbers	Prefixes	Stem	
Locates the	Substituents in alphabetical order	The name of the	ldentifes the
substituents in		pricipal (longest)	principal
the molecule		chain	functional group

The Principal Functional Group (PFG) whose suffix name is used is selected from Table 2 The list is in order of **decreasing** priority.

Table 2.	Table 2.         Table of Functional Groups (descending order of priority)			
	Class	Formula	Prefix	Suffix
	Cation	$-NR_3^+$	ammonio-	-ammonium
Carl	ooxylic acid	-COOH	carboxy-	-oic acid
Su	lfonic acid	-SO₂OH	sulfo-	-sulfonic acid
Salt of 0	Carboxylic Acid	-COO <sup>-</sup> M <sup>+</sup>	carboxylato-	cation nameoate
	Ester	-COOR	R-oxycarbonyl-	Roate
Ac	cid Halide	−c-x o	haloformyl-	-oyl halide
	Amide	C-NH <sub>2</sub> 0	carbamoyl-	-amide
	Nitrile	−c≡n	cyano-	-nitrile
Ą	ldehyde	—С-Н Ö	formyl-	-al
	Ketone	−c− o	OXO-	-one
	Alcohol	-OH	hydroxy-	-ol
	Thiol	-SH	mercapto-	-thiol
	Amine	-NH <sub>2</sub>	amino-	-amine
	Imine	=NH	imino-	-imine
	Ether	-OR	R-oxy-	-
ТТ	hioether	-SR	R-thio-	-

Wherever "R" appears in the prefix or suffix table then the group name (*i.e.* alkyl, alkenyl, etc.) for the R group is used.

#### **Choosing the Principal Chain** Α.

The Principal Chain is chosen according to the following rules, applied in order:

- The chain must contain the (maximum number of) principal functional group(s); (a) then
- (b) it must contain the maximum number of double and triple bonds; then
- (C) it must be the longest possible carbon chain (the carbons of the -CO<sub>2</sub>H, -CEN, -C(=O)H etc. groups are counted when they form part of the principal chain).

#### Naming the Principal Chain В.

The principal chain is named after the alkane having the same number of carbon atoms, and is modified when unsaturated by the replacement of "ane" by "en(e)", "envn(e)", "adiene", etc. The final "e" of the name is omitted before "v" or a vowel (e.a. methaneol becomes methanol).

#### C. Numbering the Principal Chain

The principal chain is numbered according to the following rules, taken in order:

- (a) the PFG.'s must be given the lowest possible numbers; then
- (b) the double and triple bonds must be given the lowest possible numbers; then
- the remaining functional groups and substituents must be given the lowest (c) possible numbers.

The following example illustrates the basic approach to naming:

HO – CH <sub>2</sub> – CH – C L CH <sub>3</sub>	$CH = C - C - CH_3$ I = II CI = O	
Principal group	C  O	-one
Principal chain	$\mathbf{C} - \mathbf{C} - \mathbf{C} - \mathbf{C} - \mathbf{C} - \mathbf{C}$	hexane
Principal chain name plus principal group	0-C-C-C-C-C 0	2-hexanone
Modified name ("ane" becomes "en")	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3-hexen-2-one
Prefixes (alphabetical with location number)	— СІ — ОН — СН <sub>3</sub>	3-chloro 6-hydroxy 5-methyl

Complete name: 3-chloro-6-hydroxy-5-methyl-3-hexen-2-one

#### (ii) Naming Various Classes of Organic Compounds

#### Α. Ethers and Thioethers

In the naming of ethers as **alkyloxy** derivatives of alkanes, it is general practice to shorten the names of compounds containing four or less carbons to alkoxy derivatives (i.e., omit the syllable "-yl-"), e.g., methyloxy becomes methoxy, ethyloxy becomes ethoxy, but pentyloxy (for CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>O-) is correct.

An alternative system for naming ethers (or thioethers) is to name the alkyl groups on oxygen (sulfur) and list them in alphabetical order as separate words before the name "ether" (or sulfide).

### Examples

$CH_3 - CH_2 - O - CH_2 - CH_3$	diethyl ether or ethoxyethane
СН <sub>3</sub> СН <sub>3</sub> -СН-О-СН <sub>3</sub>	isopropyl methyl ether or 2-methoxypropane
CH <sub>3</sub> -CH <sub>2</sub> -CH <sub>2</sub> -S-CH <sub>2</sub> -CH <sub>3</sub>	ethyl propyl sulfide or 1-ethylthiopropane

#### В. Alcohols and Thiols

(a)	-OH or -SH	as the princi	ple functional group
-----	------------	---------------	----------------------

#### Examples

CH <sub>3</sub> -	OH	methanol
CH <sub>3</sub> -	SH	methanethiol
CH   CH <sub>3</sub> -CH	H₃ 1−OH	2-propanol
СН <sub>2</sub> -СН <sub>2</sub> - И ОН	СН <sub>2</sub> -СН <sub>2</sub>   ОН	1,4-butanediol
CH₂−CH └ SH	l₂−CH₂ └ SH	1,3-propanedith
CH <sub>3</sub> -CH=	CH-CH <sub>2</sub> OH	2-buten-1-ol
$\frown$	-SH	cyclohexanethi

edithiol

ethiol

# (b) -OH or -SH as other than the principle functional group

### Examples

$$\begin{array}{c} \mathsf{CH}_2-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{C}-\mathsf{H}\\ \overset{|}{\mathsf{OH}}& \mathsf{O} \end{array} \qquad 5\text{-hydroxypentanal}\\ \mathsf{CH}_3-\mathsf{CH}_2-\mathsf{CH}-\mathsf{CH}=\mathsf{CH}-\mathsf{C}-\mathsf{OH}\\ \overset{|}{\mathsf{OH}}& \overset{|}{\mathsf{O}} \end{aligned} \qquad 4\text{-hydroxy-2-hexenoic acid}\\ \begin{array}{c} \mathsf{CH}_2-\mathsf{CH}_2-\mathsf{CH}_2\\ \overset{|}{\mathsf{OH}}& \overset{|}{\mathsf{SH}} \end{aligned} \qquad 3\text{-mercapto-1-propanol} \end{array}$$

# Alcohol and Thiol Salts

The salts of alcohols and thiols are most simply named by adding "-ate" after the "-ol" of the name. Alternatively, the alcoholates may be named as alkyloxides (dropping the "yl" syllable for the first four members as in ether naming).

# Examples

 $CH_3 - O^- Na^+$  sodium methoxide or sodium methanolate  $CH_3 - CH_2 - CH_2 - CH_2 - O^- K^+$  potassium pentyloxide or potassium pentanolate

# C. Acids, Salts of Acids and Acid Anhydrides

Carboxylic acids are named by identifying the longest carbon chain containing the carboxylic acid functional group and using this carbon chain as the stem for the carboxylic acid name. The ending "-anoic acid" is added to the stem to indicate that the compound is a carboxylic acid.

## Examples

Table 3 lists the carboxylic acids that have have special (trivial) names *which are preferred* to the formal (systematic) names.

Table 3. Special Names of Co	ommon Carboxylic Ac	ids
Formula	Trivial Name	Systematic Name
H-C-OH    0	formic acid	methanoic acid
СН <sub>3</sub> -С-ОН    О	acetic acid	ethanoic acid
СН <sub>3</sub> -СН <sub>2</sub> -С-ОН    О	propionic acid	propanoic acid
$CH_3 - CH_2 - CH_2 - C - OH$	butyric acid	butanoic acid
HO – C – C – OH       O O	oxalic acid	ethanedioc acid
$\begin{array}{c} HO-C-CH_2-C-OH\\ \overset{  }{O}&\overset{  }{O}\\ O\end{array}$	malonic acid	propanedioic acid
$\begin{array}{c} HO-C-CH_2-CH_2-C-OH\\ \\ II\\ O\\ O\\ O \end{array}$	succinic acid	butanedioic acid
н соон Ж ноос н	fumaric acid	<i>E</i> -butenedioic acid
н н	maleic acid	Z-butenedioic acid
СН <sub>3</sub> -СН-С-ОН      ОН 0	lactic acid	2-hydroxypropionic acid

The stem name formed by removal of "-ic" from the trivial name is also used in naming other acid derivatives and aldehydes.

Acid anhydrides are named when symmetrical by replacement of the word "acid" by anhydride. When unsymmetrical, the two acid groups are named as separate words in alphabetical order and the word anhydride is added.

# Examples

Acid salts are named by replacicing the "ic" ending of the acid name with "ate".

# Examples

 $CH_{3}-CH_{2}-CH_{2}-C-O^{-} Na^{+}$  sodium butyrate  $CH_{3}-C-O^{-} NH_{4}^{+}$  ammonium acetate

$$CH_{3}$$
  
 $CH_{3}-C-CH_{2}-CH_{2}-CH_{2}-C-O^{-}K^{+}$  potassium 5,5-dimethylhexanoate  
 $CH_{3}$   
 $Ca^{2^{+}}(HCO_{2})_{2}$  calcium formate (or calcium diformate)

# (1002)2

# D. Esters

The alkyl (alkenyl etc.) group on oxygen is named as a separate word and is followed by the acid salt name ("-ic acid" becomes "-ate").

### Examples

$$CH_{3} - CH_{2} - C - O - CH_{2} - CH_{3}$$
 ethyl propionate  
$$H - C - O - CH_{2} - CH_{3}$$
 propyl formate  
$$\bigcup_{i=1}^{n}$$

$$CH_3 - CH_2 - CH_2 - C - O - CH - CH_3$$
 isopropyl butyrate

# E. Acid Halides

Acid halides are maned by replacing the "-ic acid" ending of the parent carboxylic acid with "-yl halide".

# Examples

$$\begin{array}{c} CH_{3}-C-CI & \text{acetyl chloride} \\ CH_{3}-CH_{2}-C-Br & \text{propionyl bromide} \\ CH_{3}-CH_{2}-CH_{2}-\overset{CH_{3}}{\overset{CH_{3}}{\overset{CH_{3}}{\overset{CH_{2}-CH_{2}-C}{\overset{CH_{3}}{$$

## F. Amides

Primary amides are named by identifying the carboxylic acid from which the amide is derived and replacing the "-ic acid" or "-oic acid" ending of the parent carboxylic acid name with the ending "-amide".

When there are substituents on the N atom, these are named using N-alkyl or N, N-dialkyl as prefixes (note N or N, N are italicised) immediately before the main chain name.

## Examples

## G. Nitriles

The nitriles formed from acids with trivial names are named by replacing the "ic acid" ending of the parent carboxylic acid with "-onitrile". Otherwise, "-nitrile" is used as a suffix to the stem name of the parent alkane.

# Examples

CH<sub>3</sub>-CN

acetonitrile

CH<sub>3</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CN heptanenitrile

$$\begin{array}{c} CH_{3} \\ CH_{3} - \overset{I}{C} - CN \\ OH \end{array} & 2-hydroxy-2-methylpropanenitrile \\ CH_{3} - CH_{2} - CH_{2} - \overset{I}{C}H - CN \\ H - CN \end{array} & 2-chloropentanenitrile \\ hydrogen cyanide (not formonitrile) \end{array}$$

**Special Note**: The prefix "cyano" is only used when a functional group of higher priority is present.

CH<sub>3</sub>CH<sub>2</sub>-CH-CH<sub>2</sub>-COOH <sup>3</sup>-cyanopentanoic acid

 $\begin{array}{c} \text{NC-CH}_2 - \begin{array}{c} \text{C} - \text{OCH}_3 \end{array} \qquad \begin{array}{c} \text{methyl cyanoacetate} \\ \\ \\ \\ \\ \\ \\ \end{array} \end{array}$ 

## H. Aldehydes

Aldehydes formally derived from acids having a trivial name are named by adding "-aldehyde" to the trivial stem (see Section 3), otherwise the suffix "-al" is used.

### Examples

$$H-C-H$$

$$O$$

$$CH_{3}-C-H$$

$$O$$

$$CH_{3}-CH_{2}-CH_{2}-C-H$$

$$O$$

formaldehyde

acetaldehyde

$$CH_{3}-CH_{2}-$$

#### Special Note: the compound

$$H - C - C - H$$
 has the special name glyoxal  
 $\| \|$   
 $O$ 

**Special Note**: The prefix "formyl" is only used when a functional group of higher priority is present.

$$\begin{array}{c} H-C-CH_2-CH_2-CH_2-CH_2-C-OH \\ \parallel \\ O \\ -C-CH_2-CH_2-CH_2-CH_2-CH_2-N(CH_3)_3 Br^{-} \end{array} \begin{array}{c} 5 \text{-formylpentanoic acid} \\ (4 \text{-formylbutyl}) \text{trimethylammonium} \\ \text{bromide} \end{array}$$

Derivatives of aldehydes and ketones, *e.g.* oximes or hydrazones are named simply by adding the word oxime *etc.* after the aldehyde or ketone name.

# Examples

Н

$$\begin{array}{ccc} CH_{3}-CH_{2}-CH_{2}-C-H & \mbox{butyraldehyde oxime} \\ & & \\ & & \\ & & \\ CH_{3}-C-CH_{3} & \mbox{acetone oxime} \\ & & \\ &$$

### I. Ketones

Ketones are named by adding the suffix "-one" to the stem of the parent carbon chain.

#### Examples

$$CH_{3}-C-CH_{2}-CH_{3}$$

$$CH_{3}-CH_{2}-C-CH_{2}-CH_{3}$$

$$CH_{3}-CH-CH_{2}-C-CH_{2}-CH_{3}$$

$$CH_{3}-CH-CH_{2}-C-CH_{2}-CH_{3}$$

$$CH_{3}-C-CH_{2}-CH_{2}-CH_{2}-C-CH_{3}$$

$$CH_{3}-C-CH_{2}-CH_{2}-CH_{2}-C-CH_{3}$$

$$CH_{3}-C-CH_{2}-CH_{2}-CH_{2}-C-CH_{3}$$

$$CH_{3}-C-CH_{2}-CH_{2}-CH_{2}-C-CH_{3}$$

butanone

3-pentanone

cyclopentanone

5-methyl-3-hexanone

2,6-heptanedione

4-ethylcyclohexanone

## Special Note: the following compounds have special names:

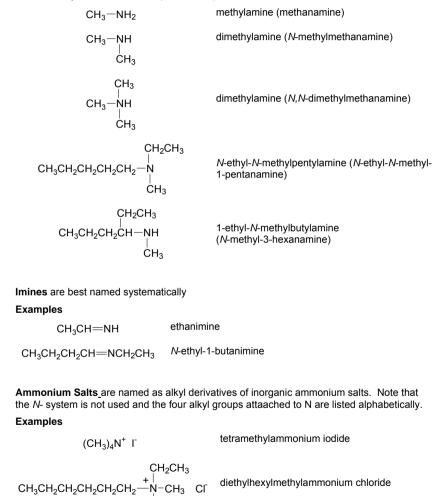
$$\begin{array}{c} \mathsf{CH}_3 - \mathsf{C} - \mathsf{CH}_3 & \text{acetone} \\ & & \mathsf{O} \\ \mathsf{CH}_3 - \mathsf{C} - \mathsf{C} - \mathsf{CH}_3 & \text{biacetyl} \\ & & \mathsf{H} & \mathsf{H} \\ & & \mathsf{O} & \mathsf{O} \end{array}$$

**Special Note**: The prefix "oxo" is used when the ketone is not the principal functional group. **Examples** 

J. Amines and Ammonium Salts

The systematic method of naming amines, whereby "-amine" is added to the principal chain name is, in practice, only rarely used and an older method is in common (I.U.P.A.C. accepted) use. Amines are named as derivatives of ammonia. The longest chain attached to the nitrogen atom is named in the usual way for an alkyl group (the carbon attached to the nitrogen is carbon 1). Any other N-substituents are named as *N*-alkyl, or *N*,*N*-dialkyl substituents. The alkyl name for the longest stem is then added to the suffix "amine".

**Examples** The following examples show this common naming in practice (together with the formal, systematic names in parenthesis):



CH<sub>2</sub>CH<sub>3</sub>

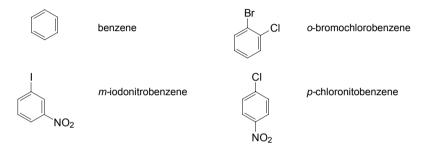
# 5 AROMATIC COMPOUNDS

# (i) General Notes

The use of numbers to indicate the position of substituents on aromatic rings is supplemented in the case of disubstituted derivatives of **benzene** by the terms:

- ortho- abbreviated o- indicating 1,2-disubstitution
- meta- abbreviated m- indicating 1,3-disubstitution
- para- abbreviated p- indicating 1,4-disubstitution

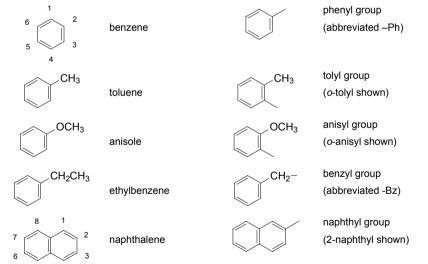
# Examples



# (ii) Aromatic Hydrocarbons

5

The following aromatic compounds have the special name and derived group names shown below:

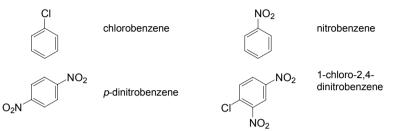


(iii) Substituted Aromatic Compounds

# A. Halogen and Nitro- Substituted Aromatics

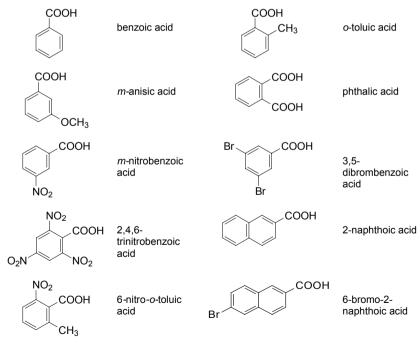
These are named using halo- or nitro- prefixes before the name of the aromatic **hydrocarbon** in the usual way.

# Examples



# B. Carboxylic Acids and Derivatives

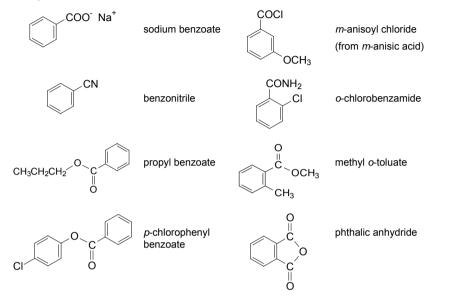
The following list gives the trivial (usually accepted) names for some of the common aromatic acids and derivatives.



# **Carboxylic acid Derivatives**

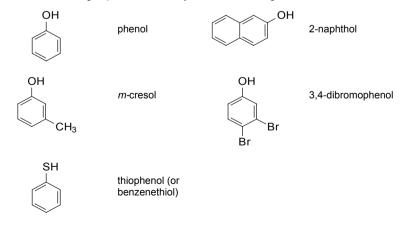
Acid derivatives, esters, anhydrides, amides and nitriles are named in the usual way, replacing "-oic" or "-ic" of the acid name with the appropriate endings.

# Examples

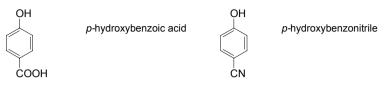


# C. Phenols and Thiophenols

Phenols have an -OH group attached directly to an aromatic ring.

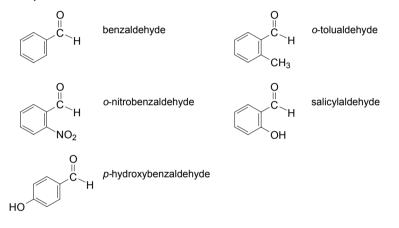


When the -OH group is not the principal functional group, "hydroxy" is used in the usual way. **Example** 



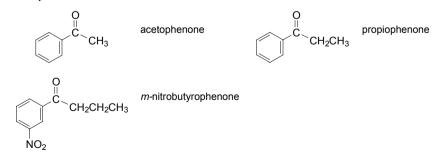
#### D. Aldehydes and Ketones

Aldehydes are named by replacing the "-ic" or "-oic" of the acid name by "aldehyde". **Examples** 



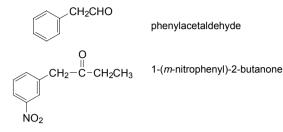
Aromatic ketones are named by changing the "ic" or "oic" ending of the acid name corresponding to the acyl group attached to the benzene ring to "-ophenone"

#### Examples



Aldehydes and ketones in which the carbonyl group is not directly attached to the aromatic ring are named using the corresponding group name for the aromatic system as a prefix.

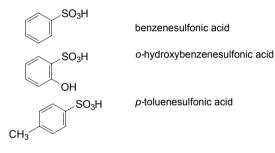
## Examples



# E. Sulfonic Acids and Sulfonic Acid Derivatives

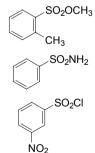
Sulfonic acids are named by adding the suffix "-sulfonic acid".

# Examples



**Sulfonic Acid Derivatives.** Derivatives of sulfonic acids (esters, amides and sulfonic acid chlorides) are named by analogy with carboxylic acids.

# Examples



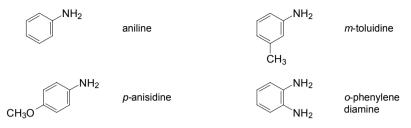
methyl o-toluenesulfonate

benzenesulfonamide

*m*-nitrobenzenesulfonyl chloride

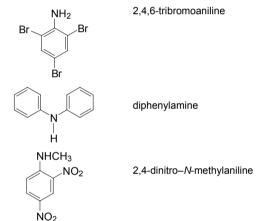
F. Aromatic Amines

# Special Names



The remaining aromatic amines are named as derivatives of these or (in the presence of more important functional groups) as "amino-" derivatives, or as "phenylamines".

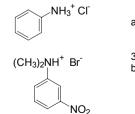
# Examples



Ammonium Salts

These are named by changing the "-e" of the special names to "-ium".

# Examples



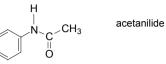
anilinium chloride

3-nitro-*N,N*-dimethylanilium bromide.

# Acyl Derivatives (Amides)

Simple acyl derivatives are named by adding the trivial acid name stem to "-anilide" etc.

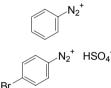
## Example



# G. Diazonium lons (ArN<sub>2</sub><sup>+</sup>)

These are named in an analogous fashion to sulfonic acids; the syllable "-diazonium" is added to the aromatic name.

# Examples



benzenediazonium ion

*p*-bromobenzenediazonium hydrogen sulfate

# 6. RADICOFUNCTIONAL NAMING

An alternate system of naming, which is still very common in many textbooks, consists of naming the alkyl or aryl groups attached to a certain functional group as separate words followed by the functional group name. The alternative naming of ethers and amines is a remnant of this system. The following examples suffice to illustrate the system.

# A. Alkyl Halides

CH <sub>3</sub> —I	methyl iodide	(CH <sub>3</sub> ) <sub>2</sub> CHBr
(CH <sub>3</sub> ) <sub>3</sub> CCl	tert-butyl chloride	CH <sub>2</sub> C

CH<sub>2</sub>CI benzyl chloride

(CH<sub>3</sub>)<sub>3</sub>COH

isopropyl

bromide

tert-butyl alcohol

# B. Alcohols



methyl alcohol



benzyl alcohol

#### C. Ketones CH<sub>3</sub>CH<sub>2</sub>C ethyl methyl CH<sub>3</sub> ∠CH<sub>3</sub> CH<sub>3</sub> ketone dimethyl ketone Ô Ô methyl vinyl C $\cap$ ketone methyl phenyl ketone CH<sub>2</sub>=CH-CH-CH<sub>3</sub> C CH<sub>3</sub> Nitriles (Cyanides) D. methyl cyanide CH<sub>3</sub>CN CH<sub>2</sub>CN benzyl cyanide Ε. **Grignard Reagents** ethyl magnesium phenyl CH<sub>3</sub>CH<sub>2</sub>MgBr MgCl bromide magnesium chloride

Revised and updated Professor L D Field May 2004