

# NAMING ORGANIC COMPOUNDS

**A GUIDE TO THE  
NOMENCLATURE USED IN  
ORGANIC CHEMISTRY**

*E. H. Tinley*

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A short series of articles by the author, published originally in *The Alchemist* (since renamed *Pharmacy Digest*), was reprinted in booklet form in 1951 with the title "A guide to the nomenclature used in organic chemistry". The kind reception given to this small booklet suggested that there was a need for such a work, and encouraged the author to produce this rather more comprehensive guide to the naming of organic compounds.

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## INTRODUCTION

**T**HE use of the term "organic chemistry" dates from the end of the eighteenth century when it referred to the study of those chemical substances which are produced during the metabolic processes of living plants and animals. It was generally believed that a *vital force* was essential for the production of these substances and that it was impossible to prepare them by the methods used for making compounds of mineral origin.

Wöhler's synthesis of oxalic acid from cyanogen in 1824, and of urea from ammonium cyanate in 1828, showed that these ideas were wrong and led eventually to the abandonment of the *vital force* theory and to the realisation that there was no justification for the original reason for treating organic and inorganic chemistry separately.

Despite the fact that the older distinction is no longer valid, it is still found convenient to make the study of organic compounds a separate branch of chemistry. There are a number of reasons for doing this but, for the present purpose, it will be sufficient to observe that since the element carbon is an essential constituent of all these compounds the term "organic chemistry" has come to mean the chemistry of the carbon compounds.

Moreover, due to the unusual facility with which the atoms of this element combine with one another to form rings and long chains, the compounds of carbon are more numerous than those of all the remaining elements.

Fortunately, the simpler carbon compounds are members of a restricted number of families.

This, together with a system of nomenclature which indicates the relationship between compounds of the same type, simplifies the study of organic chemistry.

Many problems of nomenclature have been caused by incomplete knowledge of the

structures of the substances under consideration. In these circumstances, names tended to be trivial names associated with either a method of preparation, or the reactants used, or the appearance of the product, rather than with chemical composition.

The confusion caused by such a system is exemplified by the use of the word ether. The early chemists failed to distinguish clearly between ethers and esters. They applied the term "ether" to any light, volatile, colourless liquid obtained by distilling a mixture of an acid and rectified spirit.

Amongst these substances, aether sulphuricus and aether phosphoricus (both of which consisted of diethyl ether) were obtained from rectified spirit and either sulphuric or phosphoric acid respectively, whilst aether aceticus (ethyl acetate) was prepared from rectified spirit and acetic acid. Although the correct structures had been assigned to these substances by 1850 the word ester was not used to any great extent until the beginning of this century. (Gmellin, who died in 1852, used the term *ester* in his writings, and Williamson, who was Gmellin's pupil, proved the structure of an ether proper in 1850.)

A text-book published in 1882 states categorically that both are called ethers but adds that it is necessary to distinguish between simple ethers, such as ethylic ether  $C_2H_5-O-C_2H_5$ , mixed ethers, such as methyl-ethyl ether  $CH_3-O-C_2H_5$ , and compound ethers, such as acetic ether  $C_2H_5-O-C_2H_5O$  (*sic*). This last type of compound is now called an ester.

All the British Pharmacopœias use the term Aether or Ether as principal title for ethyl ether. Aether aceticus first became the subject of a monograph in the Pharmacopœia of 1885 and this term was retained as principal title for ethyl acetate in both the 1898 and 1914 Pharmacopœias. Evidently, the pharm-

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aceutical profession is in some measure responsible for perpetuating outmoded nomenclature.

Whilst those of us who were brought up on coloured carboys, pink string, bottle caps (preferably folded by hand), sealing wax and all the other paraphernalia of our ancient craft, are loth to part either with these or our hieroglyphic though sometimes inaccurate dog-Latin, we also have a duty to see that our drugs are given names which are designed to reveal rather than to conceal their true nature.

The need for a rational system of chemical nomenclature was appreciated by many famous chemists of the late eighteenth and early nineteenth century. Among those who published papers on the subject were Bergmann, Berthollet and Lavoisier, whilst Berzelius introduced a system of symbols which forms the basis of those used in our present day chemical formulae.

Dumas also was aware of the difficulties created by the use of incorrect names. The London Pharmacopoeia 1836, in addition to describing the preparation of aether sulphuricus, has a monograph devoted to oleum aetherium. This also was made by the action of sulphuric acid on rectified spirit which were refluxed together instead of being distilled. The monograph cites an elementary analysis of the product, which was impure ethyl hydrogen sulphate ( $C_2H_5OSO_3H$ ), and quotes Dumas as "observing that if the name sulphuric aether had not been already in use, [for ethyl ether] it would be the proper appellation of aetherial oil."

The names of organic substances form an important part of the language in which organic chemists communicate with one another. Year by year, more and more new organic compounds are prepared, and organic nomenclature must be used continually to supply names for these new compounds. It is a living language and, as such, is bound to undergo continuous change both by the addition of new terms and by modification of the meanings of old ones.

Most of these alterations are to be commended, since they assist clarity of expression and help to eliminate ambiguity; but, since it would be impossible to rewrite all the older chemical literature, it is necessary to be aware of both modern and less recent usage. For this reason, the first rule of nomenclature of the International Union of Pure and Applied Chemistry (I.U.P.A.C.) states that "as few changes as possible will be made in terminology universally adopted."

In 1859, Kekulé drew attention to the importance of representing organic compounds by formulae which would indicate the way in which atoms were arranged within the molecule. His work (together with that of van't Hoff and independently of Le Bel in 1874 postulating a tetrahedral arrangement of the four valency bonds of the carbon atom) led to the development of the structural formulae which are now in use.

The importance of structural formulae lies in the fact that they summarise the chemical properties of the compound to which they relate. But, as structural formulae cannot be arranged in alphabetical order and so indexed, a method of describing organic compounds in words is necessary. This is achieved by using a systematic nomenclature. The systematic name has the advantage of being descriptive of the structure of the compound to which it applies; but it may have the disadvantage of being long and difficult to enunciate. Where compounds, such as those of the Pharmacopoeia, are in frequent use, the coining of a euphonious trivial name as a synonym must be condoned.

Reliable guidance on modern British organic nomenclature may be obtained by consulting the *Editorial Reports on Nomenclature*, which have been published annually, since 1950, by the Chemical Society. These have now been summarised in a book entitled *Handbook for Chemical Society Authors 1960*. Provided that due allowance be made for the fact that names have been adapted to the genius of a particular language, the term-

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inology of many foreign languages will be found to be similar to that described in these reports, which are based on those issued by the Commissions of Nomenclature of the I.U.P.A.C. on which most of the larger countries of the world are represented.

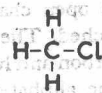
Systematic names are derived, as far as possible, by *substitutive nomenclature*; that is, an organic substance is considered to be derived by replacing one or more hydrogen atoms of a parent compound by an equal number of different atoms or groups of atoms.

The formulae of most organic compounds can be dissected into two or more parts. The more important residue—usually that of greatest molecular weight—is considered to be the parent substance, to which the smaller groups are attached as substituents. The positions which they occupy are defined by numbering the parent substance in a conventional manner.

The substance represented by the formula  $\text{CH}_3\text{Cl}$  is called monochloromethane. In this example, the parent compound is methane in which one hydrogen atom has been replaced by one chlorine atom as substituent.



Methane



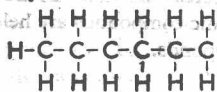
Monochloromethane  
(methyl chloride)

The alternative name methyl chloride, which is derived from the binary nomenclature of inorganic chemistry, is considered to be less correct since it implies that methyl chloride is analogous in structure to sodium chloride. This is not so, for sodium chloride molecules consist of ions bound together by electrovalencies, whereas the atoms in the molecules of most organic compounds are held together by covalent bonds.



## THE ALIPHATIC COMPOUNDS

**T**HE aliphatic compounds have an open chain of carbon atoms as skeleton. This open chain may be either straight or branched. The *paraffins*, which are composed of carbon and hydrogen only, are the simplest of the aliphatic compounds. Those which have a straight chain of carbon atoms are known as the normal paraffins and are the parents from which the nomenclature of all other aliphatic compounds is derived. The first four members of this series have trivial names—methane, ethane, propane and butane—but even these names follow the rule that the name of a paraffin ends in -ANE. The



n-Hexane

names of the remaining members of this series are composed of a prefix which indicates the number of carbon atoms in the compound, followed by the termination -ANE. Therefore, *n*-hexane is the name given to the normal paraffin having a chain of six carbon atoms.

Paraffins from which, theoretically, one atom of hydrogen has been removed, become monovalent alkyl radicals. Their names are formed by substituting the suffix -YL for -ANE in the name of the paraffin. The termination -YLIDENE is used to denote divalent radicals, obtained by removing two atoms of hydrogen from the same carbon atom.

Divalent radicals which are formed by loss of one hydrogen atom from each terminal carbon atom of a normal paraffin and which therefore consist of a chain of methylene ( $\text{CH}_2$ , <) groups, have names which specify the number of these groups in the radical. (The radical derived in this way from ethane is an exception and shares the trivial name of the first member of the olefin series.) Examples are shown in Table I.

Thus the paraffins are the saturated hydrocarbons corresponding with the alkyl radicals and the series as a whole is known as the *alkanes* (ALK-ANES).

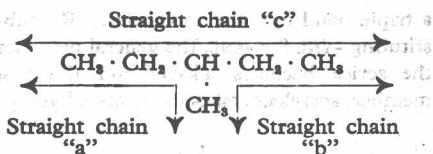
Branched chain alkanes are treated as alkyl derivatives of the straight chain compounds for they may be obtained from them, theoretically, by inserting one or more alkyl groups in place of an equal number of hydrogen atoms. The following represents an isomer of hexane:—

TABLE I

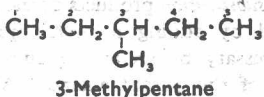
Hydrocarbon	Monovalent Radical	Divalent Radicals
$\text{CH}_4$ METHANE	$\text{CH}_3$ — Methyl	$\text{CH}_2$ < Methylene
$\text{CH}_3 \cdot \text{CH}_3$ ETHANE	$\text{CH}_3 \cdot \text{CH}_2$ — Ethyl	$\text{CH}_3 \cdot \text{CH}$ < EthYLIDENE — $\text{CH}_2 \cdot \text{CH}_2$ — Ethylene
$\text{CH}_3 \cdot \text{CH}_2 \cdot \text{CH}_3$ PROPANE	$\text{CH}_3 \cdot \text{CH}_2 \cdot \text{CH}_2$ — <i>n</i> -Propyl	$\text{CH}_3 \cdot \text{CH}_2 \cdot \text{CH}$ < <i>n</i> -PropYLIDENE — $\text{CH}_2 \cdot \text{CH}_2 \cdot \text{CH}_2$ — Trimethylene



# ALIPHATIC COMPOUNDS

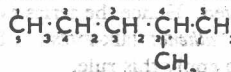


The formula of this compound contains three "straight" chains of carbon atoms, chains "a" and "b" being four carbon atoms long, and chain "c", five carbon atoms long. Of these, the last (which corresponds with the carbon skeleton of pentane) is the largest portion of the molecule. Pentane is therefore regarded as the parent hydrocarbon of the compound which is accordingly called 3-methylpentane.



Chains "a" and "b" appear in the plane formula not to be straight. This is because it is not possible to represent accurately a three-dimensional body in a two-dimensional diagram. Moreover, a so-called straight chain is in fact considerably inflected.

Another isomer of hexane is shown below:—



The figures shown above and below the carbon atoms of the pentane chain indicate that this compound could be called either 2-methylpentane or 4-methylpentane. In such cases, the name chosen is that in which the smaller numbers appear and this is a principle of general application. The correct name for this substance is therefore 2-methylpentane.

A series of compounds derived, in theory,

TABLE II

ALKANE		ALKENE ("Trivial" names in brackets)	
Ethane	$\begin{array}{c} \text{H} \quad \text{H} \\   \quad   \\ \text{H}-\text{C}-\text{C}-\text{H} \\   \quad   \\ \text{H} \quad \text{H} \end{array} \xrightarrow{-2\text{H}}$	$\begin{array}{c} \text{H} \quad \text{H} \\   \quad   \\ \text{C}=\text{C} \\   \quad   \\ \text{H} \quad \text{H} \end{array}$	Ethene (Ethylene)
Propane	$\begin{array}{c} \text{H} \quad \text{H} \quad \text{H} \\   \quad   \quad   \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{H} \\   \quad   \quad   \\ \text{H} \quad \text{H} \quad \text{H} \end{array} \xrightarrow{-2\text{H}}$	$\begin{array}{c} \text{H} \quad \text{H} \quad \text{H} \\   \quad   \quad   \\ \text{H}-\text{C}-\text{C}=\text{C} \\   \quad   \quad   \\ \text{H} \quad \text{H} \quad \text{H} \end{array}$	Propene (Propylene)
n-Butane	$\begin{array}{c} \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \\   \quad   \quad   \quad   \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H} \\   \quad   \quad   \quad   \\ \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \end{array} \xrightarrow{-2\text{H}}$	$\begin{array}{c} \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \\   \quad   \quad   \quad   \\ \text{C}=\text{C}-\text{C}-\text{C}-\text{H} \\   \quad   \quad   \quad   \\ \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \end{array}$	But-1-ene ( $\Delta^1$ -Butylene) not $\Delta^2$ -butylene
		$\begin{array}{c} \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \\   \quad   \quad   \quad   \\ \text{H}-\text{C}-\text{C}=\text{C}-\text{C}-\text{H} \\   \quad   \quad   \quad   \\ \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \end{array}$	But-2-ene ( $\Delta^2$ -Butylene)

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from the alkanes, by removing one atom of hydrogen from each of two adjacent carbon atoms and so introducing a *double bond* into the molecule, bears the trivial name *olefins*.\* The systematic names for these compounds are formed by substituting the suffix *-ENE* for *-ANE* in the name of the alkane from which they are derived. Hence the series as a whole is called the *alkenes* (alk-*ENES*). Table II shows how to apply this rule.

The symbol  $\Delta$  (delta), used as in  $\Delta^{1(2)}$ -butylene is an indication that a double bond occurs in the molecule and the figures which follow show the position of the carbon atoms between which the double bond occurs. Here again the convention of keeping the numbers as small as possible is observed and the compound is called  $\Delta^{1(2)}$ -butylene rather than  $\Delta^{3(4)}$ -butylene.

Although the symbol  $\Delta$  was used in the older literature, many recent publications omit it, and rely solely on the termination *-ENE* to show the olefinic character of a compound. The position of the double bond is then indicated by inserting a numeral in the name, immediately before the termination. This implies that the double bond is between the carbon atom thus indicated and that having the next higher number. Hence the systematic name for  $\Delta^{1(2)}$ -butylene becomes but-1-ene.

Compounds having two double bonds are classified as *dienes* (di-*enes*), those with three as *trienes* (tri-*enes*) and so on.

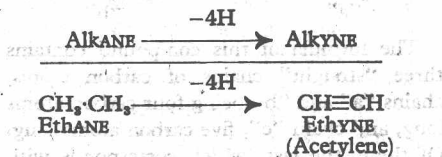
The alkenes can give rise to monovalent radicals by loss of one atom of hydrogen. Their names are formed by changing the termination *-ENE* into *-ENYL*. Thus :—

Ethene  $\text{CH}_2=\text{CH}_2$  gives rise to the eth-*ENYL*  $\text{CH}_2=\text{CH}-$  radical (which is also known by the trivial name "vinyl").

The group of hydrocarbons formerly called the *acetylenes* is derived from the alkanes by removing two hydrogen atoms from each of two adjacent carbon atoms, thus introducing

\*Often written with the less acceptable spelling *olefines*. See foot of next column for use of terminations *-IN* and *-INE*.

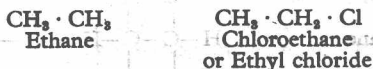
a triple bond into the molecules. By substituting *-YNE* for *-ANE*, the general name for the series becomes *alkyne* and the first member, acetylene, takes the name *ethyne*:—



Loss of one atom of hydrogen from an alkyne produces a monovalent radical named by changing *-YNE* into *-YNYL*. Thus acetylene or ethyne  $\text{CH}\equiv\text{CH}$  gives rise to the ethynyl radical  $\text{CH}\equiv\text{C}-$ .

Certain *substitution* products of the alkanes are named by adding a prefix (preceded where necessary by an arabic numeral) to the name of the parent alkane. Amongst these compounds are the chloro-, bromo-, iodo-, and nitro- ( $-\text{NO}_2$ ) derivatives.

Thus ethyl chloride, which is derived by replacing one hydrogen atom of ethane by a chlorine atom, becomes chloroethane in systematic nomenclature.



In other groups of compounds a suffix is added to the name of the parent hydrocarbon, an arabic numeral showing the position of the substituent group. Elision of the final "e" of the hydrocarbon (for the sake of euphony) is a common practice in forming names of this type.

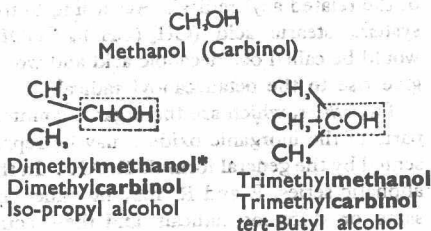
The termination *-OL* is used for *alcohols* (and *phenols*). Some examples are given in table III and it might be noted in passing that the use of the terms *glycerin* and *glycerine* for the alcoholic substance *glycerol* is to be deprecated, as the termination *-IN* should be reserved for naturally occurring fats, proteins and glycosides and *-INE* for organic bases.

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TABLE III

TRIVIAL NAME	FORMULA	SYSTEMATIC NAME
Ethyl alcohol	$\text{CH}_3 \cdot \text{CH}_2 \cdot \text{OH}$	Ethanol
<i>n</i> -Propyl alcohol	$\text{CH}_3 \cdot \text{CH}_2 \cdot \text{CH}_2 \cdot \text{OH}$	Propan(e)-1-ol
<i>iso</i> -Propyl alcohol	$\text{CH}_3 \cdot \underset{\text{1}}{\text{CH}}(\text{OH}) \cdot \underset{\text{2}}{\text{CH}_3}$	Propan(e)-2-ol
Glycerol (Glycerine)	$\begin{array}{c} \text{1} \quad \text{2} \quad \text{3} \\ \text{CH}_2 \cdot \text{CH} \cdot \text{CH}_2 \\   \quad   \quad   \\ \text{OH} \quad \text{OH} \quad \text{OH} \end{array}$	Propan(e)-1:2:3-triol
<i>tert</i> -Butyl alcohol	$\begin{array}{c} \text{OH} \\   \\ \text{CH}_3 \cdot \underset{\text{2}}{\text{C}} \cdot \underset{\text{3}}{\text{CH}_3} \\   \\ \text{CH}_3 \end{array}$	2-Methylpropan(e)-2-ol

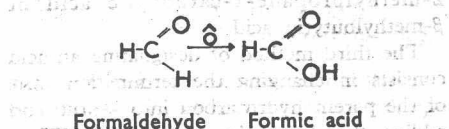
The older literature contains a number of examples of another way of dealing with *secondary and tertiary alcohols* by considering them as derivatives of methanol, which for this purpose was called "carbinol." By using this system, *iso*-propyl alcohol, which is derived by replacing two hydrogen atoms of methanol by methyl groups, became dimethylcarbinol and *tert*-butyl alcohol became trimethylcarbinol. The use of the term carbinol has now been discontinued except in a few special instances and an alcohol which was formerly called dimethylcarbinol is now described by the more readily intelligible name dimethylmethanol. Examples are given below:—



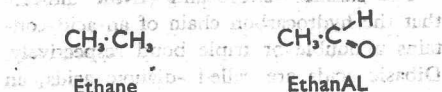
\*In this and subsequent formulae, the part of the caption in bold type corresponds to the part of the formula ringed with a dotted line.

The prefix **HYDROXY** may also be used to indicate the presence of an alcoholic group in a molecule—as for example when glycollic acid,  $\text{CH}_2(\text{OH}) \cdot \text{COOH}$ , is called hydroxyacetic acid.

The classical method of naming the aldehydes is to consider their relationship to the acids into which they are converted on oxidation. Thus formaldehyde is the aldehyde which yields formic acid.



The aldehydes are treated systematically by using the termination **-AL**. The aldehyde derived from ethane, which is commonly known as acetaldehyde, thus has the systematic name ethanal:—



## ALIPHATIC COMPOUNDS

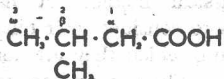
The characteristic group of all *organic acids* is the carboxyl group:—



This is often abbreviated to  $-\text{CO}_2\text{H}$  (or  $-\text{COOH}$ ) in printed articles.

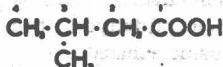
There are three ways of indicating the position of a substituent group in an acid. If it is named as a hydrocarbon-carboxylic acid, the central carbon atom, that is, the carbon atom of the carboxyl group, is not numbered, but following the usual practice, the longest hydrocarbon chain is numbered, starting with the carbon atom next to the central carbon atom.

Trivial names are acceptable for acids having five or less carbon atoms. When this system is used, the carbon atoms designated as 1, 2, etc. in the hydrocarbon-carboxylic acid system are labelled  $\alpha$ ,  $\beta$ , etc. in alphabetical order; the carbon atom which is most remote from the central carbon atom is called the omega ( $\omega$ ) carbon atom.



Applications of these rules to *iso*-valeric acid (above) shows that it may be called either 2-methylpropane-1-carboxylic acid or  $\beta$ -methylbutyric acid.

The third method of designating an acid consists in changing the termination  $-\text{ANE}$  of the parent hydrocarbon into  $-\text{ANOIC}$  and adding the descriptive word *acid*. When this system is used the central carbon atom takes the number 1 and *isovaleric acid* would then be called 3-methylbutanoic acid:—



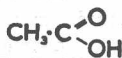
The suffixes  $-\text{ENOIC}$  and  $-\text{YNOIC}$  indicate that the hydrocarbon chain of an acid contains a double or triple bond respectively. Dibasic acids are called  $-\text{dianoic acids}$ , an

example being adipic acid which, since it is derived from *n*-hexane, takes the name hexanedianoic acid.



Hexanedianoic acid or adipic acid

Acyl radicals result from the removal, in theory, of the hydroxyl ( $-\text{OH}$ ) group from an acid. Substitution of  $-\text{YL}$  for  $-\text{IC}$  in the trivial name of a mono- or dibasic acid of low molecular weight, gives the name of the corresponding radical, but those related to the long chain fatty acids take the termination  $-\text{OYL}$ . Hence the acetyl radical is derived from acetic acid,



Acetic Acid



Acetyl radical

but stearic acid ( $\text{CH}_3 \cdot (\text{CH}_2)_{16} \cdot \text{COOH}$ ) gives rise to the stearyl ( $\text{CH}_3 \cdot (\text{CH}_2)_{16} \cdot \text{CO}-$ ) group, confusion with the stearyl ( $\text{CH}_3 \cdot (\text{CH}_2)_{17}-$ ) group being thereby avoided.

Similarly, if the acid has been named as a hydrocarbon-carboxylic acid, the word carboxylic is converted into carbonyl so that the radical derived from 2-methylpropane-1-carboxylic acid becomes the 2-methylpropane-1-carbonyl group.

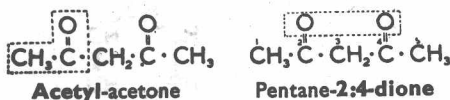
However, it is preferable to avoid this type of nomenclature, wherever possible, by naming the parent acid as an  $-\text{ANOIC}$  acid and altering this to  $-\text{ANOYL}$  to form the name of the related acyl radical. According to this system, stearic acid ( $\text{CH}_3 \cdot (\text{CH}_2)_{16} \cdot \text{COOH}$ ) would be called octadecanoic acid and would give rise to the octadecanoyl radical.

The *ethers*, which are the organic counterparts of the inorganic oxides, may be represented by the general formula  $\text{R.O.R'}$ . In the aliphatic series, R and R' may be either the same or different radicals and these compounds are conveniently named by specifying these radicals and adding the designation

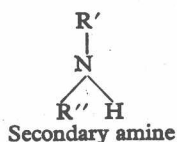
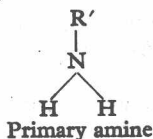
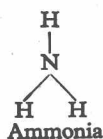
## ALIPHATIC COMPOUNDS

ether. Thus Ether B.P. which is represented by the formula  $C_2H_5 \cdot O \cdot C_2H_5$  is diethyl ether or more correctly ethyl ether, since it is customary to omit the prefix di- from the names of ethers (and ketones) which have symmetrical structures of this type. Ethers are more correctly named by considering them as alkoxyderivatives of a hydrocarbon, so that diethyl ether becomes ethoxyethane. This practice is adopted only when one of the groupings is much larger and more important than the other (as for example in mepacrine to which reference will be made later).

**Ketones** have the general formula  $R \cdot CO \cdot R'$ . They may be named in an analogous manner to the first method mentioned for ethers. The substance having the formula  $C_2H_5 \cdot CO \cdot CH_3$  is ethylmethylketone. This method cannot be applied in more complex cases, when the termination -ONE is used. Diketones are termed diones, and triketones are termed triones. This rule is illustrated by acetylacetone, the systematic name for which is pentane-2:4-dione :—

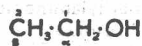


**Organic derivatives of ammonia** are designated primary, secondary and tertiary amines according to the number of hydrogen atoms of ammonia which have been replaced by organic groups.

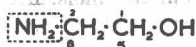


Their names are obtained, either by com-

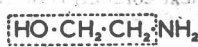
bining those of the substituent groups with the termination -AMINE or by using the prefix AMINO- in conjunction with the name of the other portion of the molecule. Ethanolamine or  $\beta$ -aminoethanol is a primary amine obtained, theoretically, by substituting a primary amino-group ( $-NH_2$ ) for one hydrogen atom on the  $\beta$  carbon atom of ethanol. Some authorities prefer to use arabic numerals rather than Greek letters to show the positions of substituent groups and this compound may be called 2-aminoethanol, thus :—



Ethanol



$\beta$ -Aminoethanol  
2-Aminoethanol

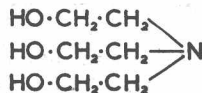


Ethanolamine

In triethanolamine, which is a tertiary amine, all three hydrogen atoms of ammonia have been replaced by ethanol residues which are also termed 2-hydroxyethyl groups.



Ammonia

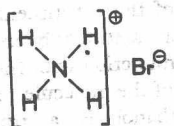


Triethanolamine  
or Tri-(2-hydroxyethyl)-amine

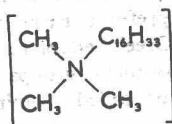
The alkaloids are substances of diverse structure which resemble one another, slightly, in being amines or organic bases. Their basic nature is indicated by making their trivial names end in -INE.

**Quaternary ammonium compounds** are derived from salts of the ammonium radical by replacing the hydrogen atoms by alkyl groups. The chief constituent of cetrimide is cetyltrimethylammonium bromide, that is, ammonium bromide in which three of the hydrogen atoms are replaced by methyl groups, the fourth being replaced by a cetyl (hexadecyl) group.

# ALIPHATIC COMPOUNDS



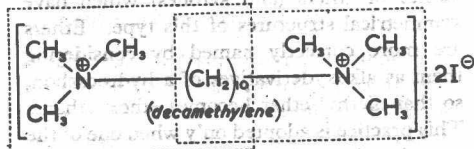
Ammonium  
bromide



Cetyltrimethylammonium  
bromide

Decamethonium iodide (see formula in next column) is derived from two molecules

of ammonium iodide as indicated by the dotted lines. It is called decamethylene-1:10-bistrimethylammonium di-iodide. The



Decamethonium iodide

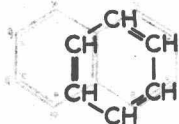
syllable *bis* is indicative of the two ammonium residues present in the molecule. The structure of the ammonium radical is discussed further in the section dealing with the stereo chemistry of the oximes (see p. 34).

## THE HOMOCYCLIC COMPOUNDS

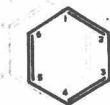
**B**ENZENE, which has the molecular formula  $C_6H_6$ , has a skeleton of six carbon atoms arranged in a closed ring. Armstrong suggested that benzene be represented by a regular hexagon. This symbol, which had the merit of ignoring any controversy as to the actual arrangement of the valency bonds, is found in most of the older literature. Modern usage requires that the symbol should be drawn with alternate single and double bonds in order to emphasise the "aromatic" nature of the compound. These symbols together with Kekulé's formula for benzene are shown below :—



"Armstrong" symbol for benzene



"Kekulé" formula for benzene



Modern symbol for benzene

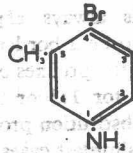
Derivatives of benzene are obtained by replacing one or more of the hydrogen atoms by substituent atoms or groups. As all six positions in the benzene nucleus are equivalent, there can be no ambiguity with *mono*-substitution products.

In order to indicate the structure of more highly substituted derivatives, the benzene ring is numbered from one to six in either a clockwise or an anticlockwise direction. It was customary, formerly, to mention substituents in a recognised order of precedence irrespective of the position which they occupied in the molecule. In 1950, the Chemical Society discontinued this practice in favour of an alphabetical order, the

functional group being assigned position 1 as shown in the following examples :—



4-Methylphenol  
(*p*-cresol)



4-Bromo-2,5-  
dimethylaniline

When more than one functional group is present in any compound (either open-chain or cyclic) the lowest number is assigned to the principal function, which is expressed by a suffix.

All the other functional groups are denoted by prefixes. A note in the Editorial Report on Nomenclature 1952 appended to rule 51 of the I.U.P.A.C. gives a list of functional groups in order of precedence (see Appendix I) and this order should be followed unless it is necessary, for a particular purpose, to emphasise that some other functional group is present.

This is illustrated by the following example :—The phenolic function normally takes precedence over the amino-function and the compound represented by the following formula should be called 4-amino-



phenol. If its properties were being compared with those of a series of amines, the amino-function would be more important from the point of view of this particular discussion. It would then be permissible and indeed preferable to call it 4-hydroxyaniline.

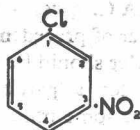
The term "functional group" cannot be



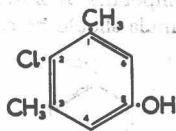
## HOMOCYCLIC COMPOUNDS

defined precisely, but may be taken to mean any group which confers characteristic properties on a compound. Thus the carboxylic acid and ketonic groups are definitely functional, whilst methyl and phenyl are non-functional; but the chloro-group (which is always expressed by a prefix) appears to be a borderline case.

Use of the prefixes *ortho* (*o*) for 1:2 or 1:6, *meta* (*m*) for 1:3 or 1:5, and *para* (*p*) for 1:4-di-substitution products is satisfactory in only the simplest cases. This can be seen by comparing the application of this method to *m*-chloronitrobenzene (1-chloro-3-nitrobenzene) and to *p*-chloro-*m*-xynol (2-chloro-5-hydroxy-1:3-dimethylbenzene). In applying the rule relating to alphabetical order of substituents, syllables such as "di" are ignored. Thus "hydroxy" comes before "dimethyl" in the systematic name just mentioned.



*m*-Chloronitrobenzene  
or  
1-chloro-3-nitrobenzene

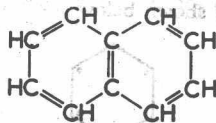


*p*-Chloro-*m*-xynol  
or

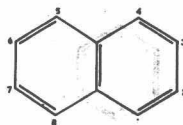
2-chloro-5-hydroxy-1:3-dimethylbenzene

The "Kekulé" structure of naphthalene and the derived symbols together with the conventional system of numbering are shown below. The double bonds, which were omitted in the older literature, should be inserted in the formula to indicate the aro-

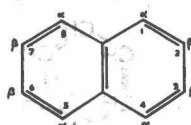
matic nature of the substance and the similarity of its properties to those of benzene. Positions 1, 4, 5 and 8, which are obviously equivalent, are designated  $\alpha$  (alpha) positions. They differ from positions 2, 3, 6 and 7 which are equivalent  $\beta$  (beta) positions. Here again the use of  $\alpha$  and  $\beta$  is satisfactory only for the simplest derivatives. (Symbols I and II are identical for they may be superimposed by rotating one of them through  $180^\circ$  perpendicularly out of the plane of the paper). The "Kekulé" formula for naphthalene shows that it is not possible to obtain a substitution product on the carbon atoms in the re-entrant angles; therefore these positions are not numbered.



"Kekulé" formula for naphthalene

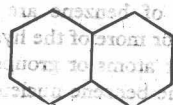


(I)



(II)

Modern symbols for naphthalene



"Armstrong" symbol for naphthalene

The method of naming betanaphthol (which is a phenolic derivative of naphthalene) will be apparent from the formula :



$\beta$ -Naphthol or 2-naphthol

## HOMOCYCLIC COMPOUNDS

Acetomenaphthone is obtained by acetylation of 1:4-dihydroxy-2-methylnaphthalene. The hydrogen atom of each hydroxyl group

is thus replaced by an acetyl group and the product is therefore 1:4-diacetoxy-2-methylnaphthalene (see equation below).

