SECTION 6

NOMENCLATURE AND STRUCTURE OF ORGANIC COMPOUNDS

Greek and Latin prefixes play an important role in nomenclature:

	Greek	*Latin*
½	hemi	semi
1	mono	uni
1½		sesqui
2	di	bi
3	tri	ter
4	tetra	quadri
5	penta	quinque
6	hexa	sexi
7	hepta	septi
8	octa	octo
9	ennea	nona
10	deca	deci

Organic compounds: Compounds containing the element carbon [e.g. methane, butanol]. (CO, CO_2 and carbonates are classified as inorganic.) See *page 1-4*.

Special characteristics of many organic compounds are chains or rings of carbon atoms bonded together, which provides the basis for naming, and the presence of many carbon-hydrogen bonds. The valency of carbon in organic compounds is 4.

Hydrocarbons: Compounds containing only the elements C and H.

Straight chain hydrocarbons are named according to the number of carbon atoms: CH_4, methane; C_2H_6 or $H_3C\text{-}CH_3$, ethane; C_3H_8 or $H_3C\text{-}CH_2\text{-}CH_3$, propane; C_4H_{10} or $H_3C\text{-}CH_2\text{-}CH_2\text{-}CH_3$, butane; C_5H_{12} or $CH_3CH_2CH_2CH_2CH_3$, pentane; C_6H_{14} or $CH_3(CH_2)_4CH_3$, $_9H_{20}$, nonane; $C_{10}H_{22}$, $CH_3(CH_2)_8$

pent-, (5); *hex-*, (6); *hept-*, (7): *oct-*, (8); *non-*, (9); *dec-*, (10); *alk-*, general. The ending *-ane* means no **unsaturation** (no double or triple bonds). Alkanes may be non-cyclic (**acyclic**) or **cyclic** (contain rings). The general formula for an acyclic alkane is C_nH_{2n+2} and for one containing one ring C_nH_{2n}. In cyclic alkanes the stem gives the number of carbon atoms in the ring. [e.g. *c*-C_6H_{12} is cyclohexane, where *c*- means cyclic]

Unsaturated compound: A compound with one or more multiple (double or triple) bonds [e.g. ethene (ethylene), $CH_2=CH_2$].

Alkene: A hydrocarbon containing a double bond [e.g. C_3H_6, CH_3-$CH=CH_2$, propene].

Alkyne: A hydrocarbon containing a triple bond [e.g. C_4H_6 or $CH_3CH_2C\equiv CH$, but-1-yne]. The endings *-ene* and *-yne* are for the double or triple bond respectively. The general formula C_nH_{2n+2} loses two H's for each ring or each double bond and four H's for each triple bond. The position of the multiple bond is shown by a number in the name, numbering from the end of the chain to give the smallest number [e.g $CH_3CH_2CH_2CH=CH_2CH_2CH_3$ is hept-3-ene (formerly 3-heptene) not hept-4-ene].

Alkyl group: In general, an alkane minus one hydrogen atom and represented by R [e.g. CH_3- is methyl (sometimes shown as Me); CH_3CH_2- is ethyl (sometimes shown as Et); $CH_3CH_2CH_2$- is propyl (sometimes shown as Pr); $CH_3CH_2CH_2CH_2$- is butyl (sometimes shown as Bu)].

In straight chain alkanes the non-terminal carbon atoms are bonded to two other carbon atoms. In a <u>branched</u> alkane one or more carbons are bonded to three or four other carbon atoms.

Primary carbon atom: A carbon atom bonded to only one other C atom.

Secondary carbon atom: One bonded to two other C atoms.

Tertiary carbon atom: One bonded to three other C atoms.

Quaternary carbon atom: One bonded to four other C atoms.

Branched hydrocarbons are named after the longest chain (saturated) or the longest chain containing the double or triple bond (unsaturated) with the branched group given by its alkyl name. [e.g. $CH_3C(CH_3)_2CH_2CH_3$ is 2,2-dimethylbutane.]

Isomers: Compounds with the same molecular formula but with their atoms arranged differently [e.g. hexane and 2,2-dimethylbutane, both C_6H_{14}].

Constitutional (structural) isomers: Isomers having their atoms joined together in a different sequence. (Some chemists restrict this term for isomers which have different **functional groups** [e.g. hexene and cyclohexane]. They would classify isomers containing the same functional groups as **positional isomers** [e.g. 2-methylpentane, $CH_3CH(CH_3)CH_2CH_2CH_3$ and 3-methylpentane, $CH_3CH_2CH(CH_3)CH_2CH_3$]).

Organic compounds are classified by the **functional groups** they contain.

Functional group: An atom or group of atoms which give the compound distinctive chemical properties [e.g. -Cl, -OH, >C=C<, -CO_2H]. Thus all organic compounds except saturated hydrocarbons have one or more functional groups. The functional group determines the class of compound. In nomenclature the functional group may be identified by a prefix, a suffix, or by the class of compound. (See below)

Common functional groups and classes of compounds are:

-F, *fluoro*-; -Cl, *chloro*-; -Br, *bromo*-; -I, *iodo*-; generally called **haloalkanes** (prefix) or **alkyl halides** (class of compound). [e.g. CH_3CH_2Cl is chloroethane or ethyl chloride. $CH_3CHFCH_2CH_3$ is 2-fluorobutane or secondary butyl fluoride.]

-OH, *hydroxy*-, giving rise to **alcohols**. The -OH group can be named as the prefix *hydroxy*-, as the suffix -*ol* replacing the -*e* of the alkane or as an alcohol. [e.g. $CH_3CH(OH)CH_2CH_3$ is butan-2-ol or secondary butyl alcohol; $(CH_3)_3COH$ is 2-methylpropan-2-ol or tertiary butyl alcohol].

-NH_2, *amino*-, giving rise to **amines**. The -NH_2 group can be named as the prefix *amino*-, with the suffix -*amine* replacing the -*e* of the alkane or as an amine. [e.g. $CH_3CH_2NH_2$ is aminoethane, ethanamine or ethylamine.] Amines can be considered as ammonia with

are used in naming. [e.g. $CH_3CH_2CH_2CO_2H$ is called butanoic acid. Methanoic acid, HCO_2H, is commonly called formic acid, and ethanoic acid, CH_3CO_2H, is commonly called acetic acid.] The group is also often written as -COOH instead of $-CO_2H$. The CH_3CO- group is commonly called the acetyl group. RCO- is an acyl group.

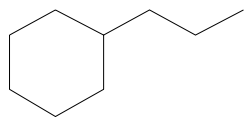
The product of the reaction of a carboxylic acid with a base is a **carboxylic acid salt**, an ionic compound. The name of the cation is given first followed by the acid with the suffix -*oate* replacing -*oic*. [e.g. $CH_3CH_2CH_2CO_2^-Na^+$ is sodium butanoate; $CH_3CO_2^-NH_4^+$ is ammonium ethanoate or ammonium acetate.] The general name for the anion is carboxylate.

When the OH of the carboxyl group is replaced by another group the compound is a **carboxylic acid derivative**. If the OH is replaced by OR of an alcohol the compound is called an **ester**. The R group is given first followed by the acid with the suffix -*oate* replacing -*oic* [e.g. $CH_3CH_2CO_2CH_2CH_3$ is ethyl propanoate]. When the OH group is replaced by NH_2 the compound is a **primary amide**. The suffix -*amide* replaces -oic. [e.g. CH_3CONH_2 is ethanamide, more commonly called acetamide]. If the OH has been replaced by an RNH the compound is a **secondary amide**, or by an RR'N group a **tertiary amide**, and the alkyl group of the amine named as such with the prefix N to show it is bonded to the nitrogen atom [e.g. $CH_3CH_2CONHCH_3$ is N-methylpropanamide]. If the OH has been replaced by a halo group the compound is an **acyl halide**, -*oic becoming -oyl* [e.g. CH_3CH_2COCl is propanoyl chloride]. If the OH has been replaced by a carboxylate group, OCOR, the compound is an **acid anhydride**. [e.g. $CH_3COOCOCH_3$ is ethanoyl anhydride or acetic anhydride. An anhydride in general is a substance formed by removing the elements of water from the compound.
[e.g. $2CH_3CO_2H \rightarrow CH_3COOCOCH_3 + H_2O$]

Multifunctional compound: A compound with more than one functional group.

Nomenclature of multifunctional compounds: The longest chain containing the suffix is chosen, the priority for choosing the suffix being carboxylic acid, $-CO_2H$, > carboxylic acid derivative, -COX > aldehyde, -CHO > ketone, -CO-, > alcohol, -OH > amine, $-NH_2$. The second and other groups are labelled as substituents. [e.g. $CH_3CH(OH)CH_2CO_2H$ is 3-hydroxybutanoic acid; $HOCH_2CH_2CH_2COCH_3$ is 5-hydroxypentan-2-one; $CH_3CH(OH)CH_2C(CH_3)(NH_2)CH_3$ is 4-amino-4-methylpentan-2-ol; CH_3COCO_2H is 2-oxopropanoic acid, (the =O of an aldehyde or ketone is called **oxo** when it has to be named as a substituent).] The carbon-carbon double and triple bonds are always incorporated in the chain, with lower priority than the other groups. [e.g. $CH_2=CHCH(OH)CH_3$ is but-3-en-2-ol; $CH_3C\equiv CCH_2CO_2H$ is pent-3-yn-oic acid.]

For compounds with larger carbon skeletons a further condensation of structural may be used.



represents propylcyclohexane. Each line represents two carbon atoms joined by a single bond, and hydrogens which are present are not shown. The number of H's is such to satisfy the valency of carbon, 4.