Second Edition

An INTRODUCTION to CHEMICAL NOMENCLATURE

R. S. CAHN

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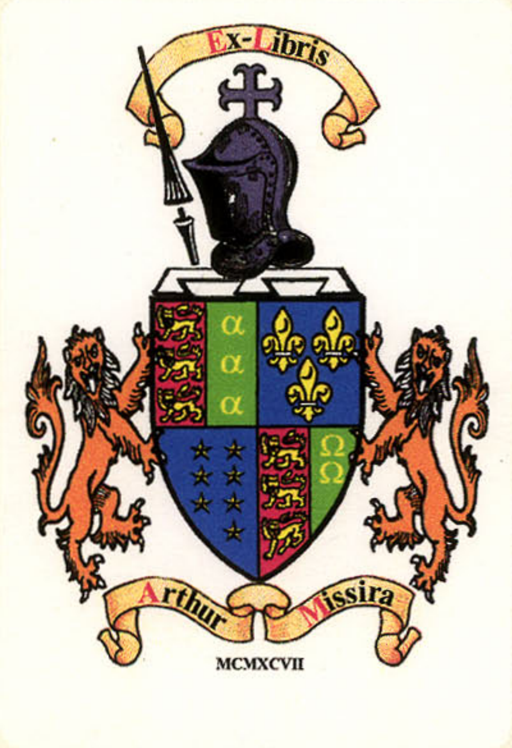

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AN INTRODUCTION
TO
CHEMICAL NOMENCLATURE

SECOND EDITION

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Introduction to Second Edition

Since the first edition, "tentative" I.U.P.A.C. rules have been published that cover characteristic (functional) groups containing carbon, hydrogen, oxygen, nitrogen, halogen, sulphur, selenium, and/or tellurium. These call for no material change in the principles described in the present elementary book, though in several matters they probe more deeply into more complex aspects. The "tentative" rules are, however, liable to amendment before being adopted as "definitive", and only on appearance of the "definitive" version can radical enlargement of the present text of this book be usefully undertaken. Such minor amendments as seemed needed have been made in the present second edition.

Most of the changes from the first edition are correction of errors (and I am grateful to the various people who pointed out errors to me), but occasional clarifications have also been made. A final chapter has, however, been added giving a few exercises with "worked" answers.

R. S. CAHN

December 1963

Introduction to First Edition

In this book I have tried to describe for chemists the principles of chemical nomenclature, particularly of modern systematic nomenclature. It is certainly not a complete textbook of nomenclature, for which the time is not yet ripe. In concentrating on principles I have limited the examples to those needed for illustration; and since nomenclature is not a subject which one normally sits down to learn systematically, whilst readers, being chemists, will know much already, I have referred whenever it was convenient to chemical matters that didactically should perhaps come later. I have also felt it right, in an "Introduction", to limit specialist points to references. Brevity has, however, not intentionally been achieved by merely omitting the harder points: I have tried always to mention any further complexities and to say where they are discussed.

Inorganic and organic chemistry have been treated differently, the former much more fully (though in less space). The 1957 I.U.P.A.C. report on inorganic nomenclature sets in parts a new pattern which is likely to remain serviceable and to guide future developments for some time ahead; the subject can be reported in an orderly way; and the innovations require rather detailed exposition, the more so as the resulting names will not always agree with those in textbooks. No such major change occurs in the postwar I.U.P.A.C. organic rules: here, however, we find a much wider field and varying methods side by side, and the main problem for the ordinary chemist is to differentiate the principles and to decide what method to use on what occasion. The full textbook to replace

Dr A. D. Mitchell's *British Chemical Nomenclature* and the Introductions to *Chemical Abstracts* indexes should wait until the work by I.U.P.A.C. on functional groups has progressed further.

The nomenclature I have recorded is, to the best of my ability, that accepted by The Chemical Society. These have been set out in detail in the "Handbook for Chemical Society Authors" (Special Publication No. 14, The Chemical Society, Burlington House, London, W.1), which should be consulted also with respect to a large number of the Society's decisions on nomenclature. I have not mentioned the changes necessary in foreign languages: but I have discussed the main differences from American practice, as these should be familiar to all who read American textbooks or *Chemical Abstracts*.

I am indebted to the International Union of Pure and Applied Chemistry and to Messrs Butterworths for permission to quote from the international reports; to Professor K. A. Jensen of Copenhagen for a copy of the latest I.U.P.A.C. Report on Inorganic Chemical Nomenclature before its publication; to my colleagues on various I.U.P.A.C. Nomenclature Commissions for long and, to me, most profitable arguments; and above all to my colleagues at The Chemical Society, Drs L. C. Cross, A. D. Mitchell, and A. E. Somerfield, for innumerable discussions.

R. S. CAHN

June 1959

1

THE USE AND MISUSE OF NOMENCLATURE

Nomenclature is the tool by which chemists describe their compounds to one another. Like other tools it can be used in several ways and it can be misused.

Chemists need to describe compounds for various purposes. According to the occasion, a scribbled structural formula, "That substance", or "compound (II)" is sometimes the most suitable designation. But lists, whether for trade or abstracts indexes or lexicons, require descriptive names; and, of course, names are essential, too, for many research papers or reports, for textbooks, and for most chemical conversation.

The nomenclature which is regarded as "correct" follows from the consensus of users' opinions. It is written in rule form by the Commissions of the International Union of Pure and Applied Chemistry, who try to see nomenclature as a whole, codifying existing practice and occasionally suggesting novelties; they accept the useful practices of specialists within their own fields but reject unnecessary aberrations from general principles.

It would be simpler if there were only one "correct" name for a substance. In practice, particularly in organic chemistry, this is not so. There are two reasons. First, large compilations such as Beilstein's *Handbuch* and *Chemical Abstracts* often use differing principles, and fundamental changes would bring chaos into their indexes; nor is a single rule feasible when two or more large sections of chemists steadfastly maintain differing customs. Secondly, in papers or textbooks it is sometimes useful to emphasize by an alternative name some structural feature involved prominently in a discussion.

In some cases, therefore, alternative names are prescribed as equally "correct" in the international rules. Then one country, Society, journal, or compendium may exercise its own preference. Within reason, each individual chemist has the same choice, though in practice he may be limited by his Society, editor, or publisher. In most cases there is one name which is correct for a particular purpose: an author may use one of the alternatives, or even an "incorrect" name, if it is essential for his theoretical arguments, but not just because of his personal "preference"; the authorized version will, with a little ingenuity, suffice for almost all purposes.

Now a systematic name for a complex compound is usually itself complex, and some thought will be needed to understand it. It is therefore misuse of nomenclature to scatter long chemical names indiscriminately into a cursive explanation of ideas (necessary though this usually is for the detailed description of an experiment). This misuse of a precision tool is far commoner than it should be: for it is better nomenclature to choose carefully a phrase such as "the unsaturated alcohol", "the derived acid", "the tricyclic ketone", "the starting material", or simply "compound (V)" than to bespatter one's prose with names such as 3β-hydroxy-5-oxo-5,6-seco-D-norcholest-9(11)-en-6-oic acid or 5-(3-diethylamino-1-methylbutyl)-1,2:8,9-dibenzacridine.

An equally common misuse is false analogy in naming new types or sub-types of compound. Here it is very hard to lay down precise rules. Selection depends on a wide knowledge of previous practice: it is only too easy to mislead—and the overriding criterion for a name is that it shall be unambiguous. The advice of the national expert or editor is here essential.

Difficulties notwithstanding, chemists should, if they wish to be clearly understood, learn to describe accurately the compounds they are handling or talking about—and a definite act of learning is needed. Nomenclature, particularly in its modern developments, is not merely an arbitrary collection of names. It combines past practice with general principles, which it is the object of the following pages to explain. Tampering with it merely makes life harder for the reader and for the searcher in indexes. It is rarely good to call a spade a shovel, with or without a prefix.

2

INORGANIC

The greater part of inorganic nomenclature was for many years handled with reasonable ease by means of the endings -ic, -ous, -ium, -ide, -ite, and -ate. When these did not suffice, help was sought mainly in prefixes of the type pyro-, hypo-, meta-, ortho-, per-, sub-, and in endings such as -oxylic, -yl, -osyl. There was, however, little consistency in the use of these adjuncts, and the resulting confusion was made worse when later studies of structure disclosed irrationalities in place of some of the supposed analogies. The Stock notation helped in many cases, and Werner's nomenclature was invaluable for co-ordination compounds.

There have been three recent international attempts to devise a general system for inorganic nomenclature. A comprehensive set of rules was issued[1] by the Commission on the Nomenclature of Inorganic Chemistry of the International Union of Chemistry* in 1940, but because of the war it received no outside comment before publication. A post-war revision was published in 1953 as "Tentative Rules"[2]; much outside comment and further consideration led to "definitive" rules resulting from the Paris Conference of 1957, which have just been issued[3]. It is this 1957 set of definitive rules which forms the basis of the present account. It will be found to involve, in places, substantial departures from the nomenclature current in textbooks and journals which precede these rules.

* The older title, International Union of Pure and Applied Chemistry (I.U.P.A.C.), was re-assumed in 1949.

The new rules legislate for many contentious points; but their chief features are acceptance of the well-known -ide nomenclature for binary compounds, recommendations for much wider use of the Stock notation, and, as an important innovation, extension of Werner's system for co-ordination compounds to a large part of general inorganic chemistry. Exceptions are still made for very common names such as water or ammonia and for a long list of acids, though the Commission doubtless hopes that these exceptions also will in time be superseded. Much that is familiar remains; and the extensions often lead to familiar or easily recognizable names such as potassium tetrachloroaurate(III) $KAuCl_4$, hydrogen dihydroxodifluoroborate $H[B(OH)_2F_2]$, potassium oxotetrafluorochromate(V) $K[CrOF_4]$; the extensions would, systematically, give disodium tetraoxosulphate for Na_2SO_4 though, of course, sodium sulphate is included among the permitted exceptions. The main virtue of the extension and revision is the replacement of personal or national preference by system and the provision of an unambiguous basis for naming new compounds.

ELEMENTS

Names and symbols for the elements are given in *Table* 1 (p. 6). Names in parentheses are those to be used with affixes, *e.g.*, cupric (not copperic), ferrate (not ironate). A few specific points may be noted. Tungsten is now accepted, after an earlier attempt to replace it by wolfram. The symbol for argon is given as Ar (not A), usage in different countries having become confused and the other rare gases having two-letter symbols. Some compounds of sulphur, nitrogen, and antimony are named by use of syllables from the Greek (thion), French (azote), or Latin

Table 1. NAMES AND SYMBOLS OF THE ELEMENTS

Name	*Symbol*	*Atomic number*	*Name*	*Symbol*	*Atomic number*
Actinium	Ac	89	Mercury	Hg	80
Aluminium	Al	13	Molybdenum	Mo	42
Americium	Am	95	Neodymium	Nd	60
Antimony	Sb	51	Neon	Ne	10
Argon	Ar	18	Neptunium	Np	93
Arsenic	As	33	Nickel	Ni	28
Astatine	At	85	Niobium	Nb	41
Barium	Ba	56	Nitrogen	N	7
Berkelium	Bk	97	Nobelium	No	102
Beryllium	Be	4	Osmium	Os	76
Bismuth	Bi	83	Oxygen	O	8
Boron	B	5	Palladium	Pd	46
Bromine	Br	35	Phosphorus	P	15
Cadmium	Cd	48	Platinum	Pt	78
Caesium	Cs	55	Plutonium	Pu	94
Calcium	Ca	20	Polonium	Po	84
Californium	Cf	98	Potassium	K	19
Carbon	C	6	Praseodymium	Pr	59
Cerium	Ce	58	Promethium	Pm	61
Chlorine	Cl	17	Protactinium	Pa	91
Chromium	Cr	24	Radium	Ra	88
Cobalt	Co	27	Radon	Rn	86
Copper (Cuprum)	Cu	29	Rhenium	Re	75
Curium	Cm	96	Rhodium	Rh	45
Dysprosium	Dy	66	Rubidium	Rb	37
Einsteinium	Es	99	Ruthenium	Ru	44
Erbium	Er	68	Samarium	Sm	62
Europium	Eu	63	Scandium	Sc	21
Fermium	Fm	100	Selenium	Se	34
Fluorine	F	9	Silicon	Si	14
Francium	Fr	87	Silver (Argentum)	Ag	47
Gadolinium	Gd	64	Sodium	Na	1
Gallium	Ga	31	Strontium	Sr	38
Germanium	Ge	32	Sulphur	S	16
Gold (Aurum)	Au	79	Tantalum	Ta	73
Hafnium	Hf	72	Technetium	Tc	43
Helium	He	2	Tellurium	Te	52
Holmium	Ho	67	Terbium	Tb	65
Hydrogen	H	1	Thallium	Tl	81
Indium	In	49	Thorium	Th	90
Iodine	I	53	Thulium	Tm	69
Iridium	Ir	77	Tin (Stannum)	Sn	50
Iron (Ferrum)	Fe	26	Titanium	Ti	22
Krypton	Kr	36	Tungsten	W	74
Lanthanum	La	57	Uranium	U	92
Lead (Plumbum)	Pb	82	Vanadium	V	23
Lithium	Li	3	Xenon	Xe	54
Lutetium	Lu	71	Ytterbium	Yb	70
Magnesium	Mg	12	Yttrium	Y	39
Manganese	Mn	25	Zinc	Zn	30
Mendelevium	Md	101	Zirconium	Zr	40

(stibium). (Two recommendations in the I.U.P.A.C. 1957 Report, namely, the use of wolframate and niccolate in place of tungstate and nickelate, have not been accepted by The Chemical Society.)

Some collective names now receive international sanction: halogens (F, Cl, Br, I, At); chalcogens (O, S, Se, Te, Po); alkali metals (Li to Fr); alkaline-earth metals (Ca to Ra); lanthanum series for elements 57–71 (La to Lu inclusive), but lanthanides only for elements 58–71 (Ce to Lu inclusive); actinium series for elements 89 (Ac) to 103, but actinides for elements whose 5*f* shell is being filled; transuranium elements for those following uranium. Compounds of chalcogens are named chalcogenides. Compounds of halogens are given as halogenides but the abbreviated form halide is likely also to continue in use. The term metalloids is vetoed.

Protium, deuterium, and tritium are retained for the hydrogen isotopes ${}^{1}H$, ${}^{2}H$, and ${}^{3}H$, respectively, but other isotopes should be designated by mass numbers, *e.g.*, oxygen-18 or ${}^{18}O$.

Indexes to be used with atomic symbols are:

left upper .	. mass number
left lower .	. atomic number
right upper .	. ionic charge
right lower .	. number of atoms

For example, ${}^{32}_{16}S^{2+}_{2}$ is a doubly charged molecule containing two atoms of sulphur, each atom having the atomic number 16 and mass number 32. These indexes need not all be inserted together; for instance, Ca^{2+} is a doubly ionized calcium ion (with natural abundance of isotopes), ${}^{15}N$ an uncharged atom of nitrogen-15, ${}^{40}K^{+}$ a singly charged ion of potassium-40. Writing the mass number as upper right index has long been the practice of most physicists, and also of most chemists in America; the physicist often needs to signify atomic attributes other than the four just listed; but the positions given above are best suited for chemists who so often need to cite both mass number and ionic charge.

Radioactivity is often indicated by an asterisk, *K; it is rarely necessary to give both the mass number and the asterisk ($*^{40}K$).

Ionic charge must be given as, *e.g.*, 2+, and not +2.

For allotropic forms of elements a very simple numerical system is recommended: monohydrogen, dioxygen, tetraphosphorus, *etc.* Trioxygen is then recommended by I.U.P.A.C. for O_3, though this can hardly be held to exclude use of the familiar name ozone since ozonide is listed among the recognized names of radicals.

Ring and chain structures can be designated by prefixes cyclo- and catena-, *e.g.*, cyclo-octasulphur (or octasulphur; for λ-sulphur), catenasulphur (or polysulphur; for μ-sulphur).

COMPOUNDS

Formulae and names should correspond to the stoicheiometric proportions, expressed in the simplest form which avoids the use of fractions (though semi and sesqui may be used for addition compounds and solvates). The molecular formula, if different, is used only when dealing with discrete molecules whose degree of association is considered independent of temperature. When there is temperature-dependence, the simplest formula is again to be used unless the molecular complexity requires particular emphasis in the context. Thus we have KCl potassium chloride, PCl_3 phosphorus trichloride, S_2Cl_2 disulphur dichloride, and $H_4P_2O_6$ hypophosphoric acid (see p. 18); NO_2 nitrogen dioxide represents the equilibrium mixture of NO_2 and N_2O_4 for normal use, but N_2O_4 dinitrogen tetroxide is used where this doubling of the formula is significant.

Names of compounds are given in two (or more) parts, the (most) electropositive constituent (cation) first and the (most) electronegative (anion) last. Exceptions are made for intermetallic compounds (below), neutral co-ordination compounds (p. 14), addenda such as solvate molecules (p. 30), and some hydrides (p. 11) (for ozone see p. 8). However, no fundamental distinction is to be made between ionized and non-ionized molecules in general.

Proportions of the various parts are expressed by Greek numerical prefixes; but there are extremely important qualifications that mono (for unity) is usually omitted and that other numerical prefixes may also be omitted if no ambiguity results. Multiplicative numerical prefixes (bis, tris, tetrakis, *etc.*) are used when followed directly by another numerical prefix and may be used in other cases where ambiguity might be caused; and prefixes may be delimited by parentheses to aid clarity further (examples are on pp. 28, 29). The terminal "a" of tetra, penta, *etc.*, is normally elided before another vowel in inorganic chemistry.

Compounds between two elements

Intermetallic compounds are normally indicated by formulae, the symbols being given in order of increasing number of the Group in the (expanded) Periodic Table (Fr, Ra, 103, Hf, Ta, W, Re, Pt, Au, Hg, Tl, Pb, Bi, Po), and within each Group in order of decreasing atomic weight (Fr, Cs, Rb, K, Na, Li, in that order before Ra, Ba, Sr, . . . , *etc.*).

In formulae and names of compounds between two non-metals that constituent is placed first which occurs earlier in the sequence:

B, Si, C, Sb, As, P, N, H, Te, Se, S, At, I, Br, Cl, O, F.

This order is arbitrary in places: it is not based solely on an order of electronegativity. The results are mostly familiar: NH_3 (not H_3N), CCl_4, NCl_3, NO, *etc.* But Cl_2O (chlorine monoxide) contrasts with O_2F (dioxygen fluoride); and the nitrogen sulphides come into use again in place of sulphur nitrides[4]. Formulae of acids such as HNO_3, H_2CO_3, $HClO_4$, H_2SO_4 are excepted from this rule.

Metals precede non-metals, in formulae and names.

When forming a complete name one leaves the name of the electropositive constituent unmodified, except when it is necessary to indicate the valency (see below); and the same applies to the name of that one of a pair of non-metals which is cited first in the list above. The name of the electronegative constituent, or of the non-metal named second, is modified to end in -ide. Normally this modification is carried out by stripping the name of the element back to the penultimate consonant and then adding "ide", as in carbon, carb, carbide; or chlorine, chlor, chloride; but the following exceptions should be noted:

bismuth, bismuthide; hydrogen, hydride;
mercury, mercuride; nitrogen, nitride;
oxygen, oxide; phosphorus, phosphide;
zinc, zincide.

When Latin names are given in *Table* 1, these are used, in the normal way.

Coupling this rule with those for numerals (p. 9), and not forgetting the provisions for omission of numerical prefixes, we then have a host of familiar names, of which the following list, based on one in the I.U.P.A.C. rules, is representative:

> sodium chloride, calcium sulphide, lithium nitride, arsenic selenide, calcium phosphides, nickel arsenide, aluminium borides, iron carbides, boron hydrides, phosphorus hydrides, hydrogen chloride, hydrogen sulphide, silicon carbide, carbon disulphide, nitrogen sulphide, sulphur hexafluoride, chlorine dioxide, oxygen difluoride, sulphur dioxide, sulphur trioxide, carbon monoxide, carbon dioxide, dinitrogen monoxide, nitrogen monoxide, dinitrogen pentoxide.

The list will be seen to cover both ionized and un-ionized compounds. (Note the hyphen used by The Chemical Society, to distinguish un-ionized from union-ized.) The compounds HHal are called hydrogen chloride, hydrogen bromide, hydrogen iodide, and hydrogen fluoride: the names hydrochloric acid, *etc.*, refer to aqueous solutions, and percentages such as 20% hydrochloric acid denote the wt./vol. of hydrogen halide in the solution (not the dilution of the concentrated acid by water).

Now, oxides could be, but are not, named by the co-ordination principle (see p. 14): *e.g.*, SO_3 is sulphur trioxide (not trioxosulphur). The same applies to peroxides, *i.e.*, compounds whose electronegative constituent is the group O_2^{2-} (when the electronegative constituents are atoms 2O or ions $2O^-$ the compounds are dioxides); for example, Na_2O_2 sodium peroxide (but PbO_2 lead dioxide).

Certain hydrides and groups of hydrides have special names, as follows:

H_2O	water	PH_3	phosphine
NH_3	ammonia	SbH_3	stibine
N_2H_4	hydrazine	Si_2H_6	disilane (*etc.*)
B_2H_6	diborane (*etc.*)*	P_2H_4	diphosphine
SiH_4	silane	As_2H_4	diarsine

---

* BH_3 has been variously called borine and borane. Borine appears preferable, because the compound is not homologous with diborane, triborane, *etc.*

Many other trivial names are abandoned in the 1957 I.U.P.A.C. rules, mostly by omission from the rules, notably those for oxides of nitrogen, and, except for custom and sentiment among the older chemists, they are little loss.

For most compounds, in most circumstances, it is unnecessary to specify valency. It can always be dispensed with when no ambiguity results, as can the numerical prefixes. So one still has very many simple names such as sodium chloride, calcium oxide, deuterium oxide, barium chloride.

When it is necessary to avoid ambiguity or desirable to aid clarity, the valency may be indicated. This can be done in three ways.

(*i*) The first way is the indirect one of using numerical prefixes which show the stoicheiometric composition, as in iron trichloride, copper dichloride, tri-iron tetroxide (though this requires the familiar juggling because the iron does not have valency 8/3).

(*ii*) When it is desired or necessary to state the actual valency, the I.U.P.A.C. rules recommend the Stock system: Roman numerals (small capitals are recommended by The Chemical Society) are placed in parentheses immediately after the name of the element concerned: they represent the oxidation number or stoicheiometric valency of the element. (For co-ordination compounds, zero is denoted by the Arabic 0.) Thus we have:

MnO_2	manganese(IV) oxide
BaO	barium(II) oxide

The rules list both English and Latin names, but favour the latter where both are given in *Table* 1; for instance:

$FeCl_3$	iron(III) chloride or ferrum(III) chloride
$CuCl_2$	copper(II) chloride or cuprum(II) chloride

(*iii*) There is of course also the much older system of denoting a higher valency state by the ending -ic, and a lower one by the ending -ous. This system is notoriously incomplete when an element can exist in more than two valency states, is not applicable to co-ordination compounds, and can be a troublesome tax on memory for the less common elements. The 1957 I.U.P.A.C. rules list the system as "in use but not recommended", stating nevertheless that it "may be retained when no more than two valencies are concerned". Probably it will die hard, for ferrous chloride comes more glibly off the older tongue than iron(II) chloride or ferrum(II) chloride, or even iron dichloride; but it probably will die, in time.

Incidentally, valent (valency) is of Latin origin, and so should be used with Latin numerical prefixes—univalent, bivalent, tervalent (or trivalent), quadrivalent, quinquevalent, sexivalent, *not* the Greek mono-, di-, tetra-, penta-, or hexa-.

Pseudo-binary compounds

A few common composite anions have names ending in -ide, namely, $-OH$ hydroxide; $-CN$ cyanide; $-NH_2$ amide; $-NH-$ imide; $-NH{\cdot}NH_2$ hydrazide; $-NH{\cdot}OH$ hydroxylamide. Treating these as the other -ide names we obtain NaOH sodium hydroxide, KCN potassium cyanide, and the like. Sodium amide ($NaNH_2$) is often abbreviated to sodamide, but there is no need to extend the practice to the analogues. Hydrogen azide seems satisfactory without recourse to the trivial name hydrazoic acid.

Allied to these anions are $-O_3$ ozonide, $-I_3$ tri-iodide, $-N_3$ azide, and $-O{\cdot}O-$ peroxide (see above). $-S_2-$ is disulphide, but in this series a practice has begun of naming compounds $HS{\cdot}[S]_x{\cdot}SH$ as sulphanes ($x=1$, trisulphane; $x=2$, tetrasulphane; *etc.*), especially for organic derivatives, by analogy with the alkanes; it has analogy, too, with the silane nomenclature which is accepted by I.U.P.A.C.[5] and it can be accepted pending confirmation of its experimental basis.

The extended co-ordination principle

In its oldest sense, the sense in which it is usually understood, a co-ordination compound is one containing an atom (A) directly attached to other atoms (B) or groups (C), or both, the number of these being such that the oxidation number of the atom (A) is exceeded.

The 1957 I.U.P.A.C. rules extend this principle by abolishing the restriction that the oxidation number must be exceeded. The effect is to bring the major part of nomenclature potentially within the scope of the nomenclature customary for co-ordination compounds. For instance, in the group SO_4, the sulphur atom is atom (A) and the oxygen atoms are (B). Even for diatomic groups such as ClO^- a "characteristic" atom (here Cl) can generally be recognized and the remainder of the nomenclature welded to that.

For discussion of this nomenclature some definitions should be noted (some will not be needed until later in this chapter, but it is convenient to group them together):

Central or nuclear atom: the atom (A) above.

Co-ordinating atom: each atom *directly* attached to the central atom.

Ligand: each atom (B) or group (C) attached to the central atom.

Multidentate ligand: a group containing more than one *potential* co-ordinating atom. Hence, unidentate, bidentate, *etc.*

Chelate ligand: a ligand actually attached to one central atom through two or more co-ordinating atoms.

Bridging group: a ligand attached to more than one central atom.

Complex: the whole assembly of one or more central atoms with their attached ligands.

Polynuclear complex: a complex containing more than one central (nuclear) atom. Hence, mononuclear, dinuclear, *etc.*

To name the complex, the names of the ligands are attached directly in front of the name of the central atom; the oxidation number of the central atom is then stated last, or the proportions of the constituents are indicated by stoicheiometric numerical prefixes; when the oxidation number is exceeded, both the numerical prefixes and the oxidation number are often needed.

The complex may be cationic, neutral, or anionic. Names of cationic and neutral complexes are not modified (except for a few mentioned below), *i.e.*, they have no characteristic ending. Names of anionic complexes are given the ending -ate, often with abbreviation.

It is very necessary to realize that according to this system the ending -ate denotes *merely* an anionic complex. When an element has variable valency this use of -ate does *not* denote a higher valency state; it is used with all valency states, the distinction between them being made by citing the oxidation number. Particular note must be taken of this because the -ate, -ite, -ide distinction is still permitted in a limited and defined, but large, number of cases, and the two nomenclatures are likely to be in use side by side for some time.

The ligands must be cited in a defined order, namely:

(*i*) anionic ligands
(*ii*) neutral and cationic ligands.

The order for anionic ligands is subdivided as follows:

(*ia*) H^-

(*ib*) O^{2-}, then OH^-

(*ic*) other anions composed of one element only, in the order given on p. 9, namely:

Te, Se, S, I, Br, Cl, O, F

where O refers to oxygen anions other than O^{2-} (*e.g.*, O_2^{2-})

(*id*) polyatomic inorganic anions: of two such anions, that containing the smaller number of atoms is cited first; and two ions containing the same number of atoms are cited in order of decreasing atomic number of the central atoms (as examples the I.U.P.A.C. text gives CO_3^{2-} before CrO_4^{2-} before SO_4^{2-}: CO_3 is here considered to be inorganic)

(*ie*) organic anions in alphabetical order.

The order for neutral and cationic ligands is:

(*iia*) water, then ammonia

(*iib*) other inorganic ligands in the sequence in which their co-ordinating elements appear in the list on p. 9, namely:

B, Si, C, Sb, As, P, N, H, Te, Se, S, At,
I, Br, Cl, O, F

(*iic*) organic ligands, in alphabetical order.

The names of most neutral and cationic ligands are used without change; those of most acidic ligands are changed to end in -o. The special regulations governing these are more conveniently discussed in appropriate places in the following sections.

Acids and normal salts containing more than two elements

Classical co-ordination compounds, that is, those where the oxidation number of the central atom is exceeded, are deferred to p. 27.

(*a*) The practices mentioned earlier hold, about citing electropositive before electronegative constituents, using Stock numbers or -ic, -ous endings, and omitting numerical prefixes and Stock numbers when no confusion arises.

For acids and salts containing more than two elements the general basis recommended by the 1957 I.U.P.A.C. rules is the extended co-ordination principle outlined in the preceding section, but there are two principal exceptions which temper the consequent break with tradition and, indeed, render the rules more an aid for difficult cases than a revolution.

(*b*) First, there is a provision that, although acids should preferably be named as hydrogen . . . ate in accordance with the general co-ordination principle, the "-ic acid" terminology is also permitted. The Commission hopes, of course, that the latter will die out, but recognizes that the change will be gradual.

Secondly, there is a list of acids, given in *Table* 2 (p. 18), which retain their "trivial" names. The list contains most of the common acids whose central atom is linked only to oxygen. It is a strictly limiting list: it must not be extended to analogous cases, except for replacement of O by S, Se, Te, or –O·O–, as mentioned below.

Anions from the acids in *Table* 2 are formed by changing -ous acid to -ite, and -ic acid to -ate, and this gives the familiar names for a further host of common compounds. For instance, $NaNO_2$ sodium nitrite and $NaNO_3$ sodium nitrate follow at once.

Na_2SO_4 sodium sulphate and Na_2CO_3 sodium carbonate follow similarly when permission to omit unnecessary prefixes (*e.g.*, from disodium sulphate) is remembered.

Table 2. TRIVIAL NAMES RETAINED FOR ACIDS

(in order of the Periodic Table)[*]

H_3BO_3	orthoboric or monoboric acid
$(HBO_2)_n$	metaboric acids
$(HBO_2)_3$	trimetaboric acid
$H_4B_2O_4$	hypoboric acid
H_2CO_3	carbonic acid
HOCN	cyanic acid
HNCO	isocyanic acid
H_4SiO_4	orthosilicic acid
$(H_2SiO_3)_n$	metasilicic acids
HNO_3	nitric acid
HNO_2	nitrous acid
H_2NO_2	nitroxylic acid
$H_2N_2O_2$	hyponitrous acid
H_3PO_4	(ortho)phosphoric acid[†]
$H_4P_2O_7$	diphosphoric or pyrophosphoric acid
$H_5P_3O_{10}$	triphosphoric acid
$H_{n+2}P_nO_{3n+1}$	polyphosphoric acids
$(HPO_3)_n$	metaphosphoric acids
$(HPO_3)_3$	trimetaphosphoric acid
$(HO)_2OP{-}PO(OH)_2$	hypophosphoric acid
$(HO)_2P{-}O{-}PO(OH)_2$	diphosphoric(III,V) acid
H_2PHO_3	phosphorous acid
$H_4P_2O_5$	diphosphorous or pyrophosphorous acid
HPH_2O_2	hypophosphorous acid
H_3AsO_4	arsenic acid
H_3AsO_3	arsenious acid
H_2SO_4	sulphuric acid
$H_2S_2O_7$	disulphuric or pyrosulphuric acid
$H_2S_2O_6$	dithionic acid
H_2SO_3	sulphurous acid
$H_2S_2O_5$	disulphurous or pyrosulphurous acid
$H_2S_2O_4$	dithionous acid
H_2SO_2	sulphoxylic acid
H_2SO_{x6} ($x > 2$)	polythionic acids
H_2SeO_4	selenic acid
H_2SeO_3	selenious acid
H_6TeO_6	(ortho)telluric acid[†]
H_2CrO_4	chromic acid
$H_2Cr_2O_7$	dichromic acid
$HClO_4$	perchloric acid
$HClO_3$	chloric acid
$HClO_2$	chlorous acid
HClO	hypochlorous acid
$HBrO_3$	bromic acid
$HBrO_2$	bromous acid
HBrO	hypobromous acid
H_5IO_6	orthoperiodic acid[‡]
HIO_4	periodic acid[‡]
HIO_3	iodic acid
HIO	hypoiodous acid
$HMnO_4$	permanganic acid
H_2MnO_4	manganic acid
$HTcO_4$	pertechnetic acid
H_2TcO_4	technetic acid
$HReO_4$	perrhenic acid
H_2ReO_4	rhenic acid

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[*] See also the text for peroxo-, thio-, seleno-. and telluro- acids.

[†] Ortho- need be used only when distinction from other acids of the series is essential.

[‡] See p. 20.

A few general principles for the use of prefixes embodied in the table may be pointed out. A prefix hypo- denotes a lower oxidation state and is used with the -ous and the -ic termination. Per- denotes a higher oxidation state, is used only with the -ic acids (and their salts), and must not be confused with peroxo- (see below). Ortho- and meta- distinguish acids of differing water content.

Thioacids are acids derived by replacing oxygen by sulphur, and are named by adding thio- before the trivial name of the acid; and seleno- and telluro- acids are treated similarly. Examples are: $H_2S_2O_2$ thiosulphurous acid (not sulphoxylic); $H_2S_2O_3$ thiosulphuric acid; KSCN potassium thiocyanate; H_3PO_3S monothiophosphoric acid; $H_3PO_2S_2$ dithiophosphoric acid; H_2CS_3 trithiocarbonic acid. However, $H_2S_2O_6$ dithionic acid and $H_2S_2O_4$ dithionous acid (not hydrosulphurous or hyposulphurous) in *Table* 2 are exceptional to this treatment, and higher homologues are named analogously.

Peroxoacids, in which –O– is replaced by –O·O–, are similarly distinguished by the prefix peroxo- (peroxy- or simply per- have frequently been used in the past), as, for example, in HNO_4 peroxonitric acid and K_2SO_5 potassium peroxosulphate, HO·O·NO peroxonitrous acid, and $H_4P_2O_8$ peroxodiphosphoric acid.

(*c*) To explain how acids and salts are named by the co-ordination method requires, first, the principles given in the preceding section and then further precision about endings.

It will be remembered that the electropositive portion is named before the electronegative, as usual, and that the electronegative, anionic portion has an ending -ate. This ending is normally added to the penultimate consonant of the name of the central atom (the Latin name being used if one is given in

Table 1), as with the -ide ending; but there are the following exceptions: antimony, antimonate; bismuth, bismuthate; carbon, carbonate; cobalt, cobaltate; nickel, nickelate; nitrogen, nitrate; phosphorus, phosphate; tungsten, tungstate; zinc, zincate.

Names for ligands (which in the simple acids now considered are all anionic) are formed by changing the endings -ide, -ite, or -ate to -ido, -ito, or -ato, respectively, for direct union to the name of the central atom; but the following do not conform:

F^-	fluoro	O^{2-}	oxo	HS^-	thiolo
Br^-	bromo	OH^-	hydroxo	S^{2-}	thio
Cl^-	chloro	O_2^{2-}	peroxo	S_2^{2-}	disulphido
I^-	iodo				

In this way $H_2[SO_4]$ becomes dihydrogen tetroxosulphate(VI); or, since the "acid" terminology is also permitted, this might become tetroxosulphuric acid. If we were to make the further provision that oxo-prefixes might be omitted when no confusion is caused, we should reach the familiar sulphuric acid; nevertheless, such argument can lead to confusion in some cases, so it is better to regard the name sulphuric acid simply as one of the permitted exceptions.

The majority of simple oxoacids are included in *Table* 2, but HIO_4 is an interesting case. By analogy with perchloric acid ($HClO_4$), this is usually called periodic acid. However, H_5IO_6 is also sometimes called periodic acid, and sometimes orthoperiodic acid. The I.U.P.A.C. Commission on the Nomenclature of Inorganic Chemistry has laid down that, to avoid confusion, HIO_4 shall be called tetroxoiodic(VII) acid and that both the names periodic and orthoperiodic acid shall apply to H_5IO_6. However, The Chemical Society has decided that in its publications the older use of periodic acid for HIO_4 shall continue and that H_5IO_6 shall be distinguished as orthoperiodic acid.

Some examples of real usefulness of the method are:

$HReO_4$	tetroxorhenic(VII) acid
H_3ReO_5	pentoxorhenic(VII) acid
H_2ReO_4	tetroxorhenic(VI) acid
$HReO_3$	trioxorhenic(V) acid
$H_4Re_2O_7$	heptoxodirhenic(V) acid

In simpler cases, it seems reasonable to omit the oxo- prefixes, as in manganic(VI) acid for H_2MnO_4, and manganic(V) acid for H_3MnO_4.

Dioxonitric(II) acid could usefully replace nitroxylic acid for H_2NO_2; and the similar names, oxonitrate(I) MNO (M = metal), trioxonitrate(II) $M_2N_2O_3$, and tetroxodinitrate(III) $M_2N_2O_4$ are recommended.

It is perhaps with the halogeno-acids that this nomenclature comes best into its own. Potassium hexachloroplatinate(IV) for K_2PtCl_6 sidesteps the older platinichloride. Chlorosulphuric(VI) acid for $H[SO_3Cl]$, *i.e.*, $Cl{\cdot}SO_3H$, where Cl could be considered to replace OH of sulphuric acid, avoids confusion with organic chemistry where replacement is normally "substitution", *i.e.*, replacement of hydrogen. Some further examples illustrate the principle:

$KAuCl_4$	potassium tetrachloroaurate
$Na[PHO_2F]$	sodium hydridodioxofluorophosphate
HPF_6	hydrogen hexafluorophosphate
$H[B(OH)_2F_2]$	hydrogen dihydroxodifluoroborate
$Na_4[Fe(CN)_6]$	sodium hexacyanoferrate(II)
$K[AgF_4]$	potassium tetrafluoroargentate(III)
$Ba[BrF_4]_2$	barium tetrafluorobromate(III)
$K[Au(OH)_4]$	potassium tetrahydroxoaurate(III)
$Na[AlCl_4]$	sodium tetrachloroaluminate
$Li[AlH_4]$	lithium tetrahydridoaluminate

If desired, the "-ic acid" alternatives could be used for the acids, and further abbreviation, as in, *e.g.*, fluorosilicate, can be made for very common compounds.

The last example in our list may come as a shock: but was not the hitherto usual lithium aluminium hydride really a negation of nomenclature? And in this connexion a little anticipation from later pages may be permitted: hydrocarbon radicals, when present as ligands, do not receive the terminal -o; so we have:

$Na[B(C_6H_5)]_4$ sodium tetraphenylborate

Ions and radicals

Anions are negatively, and cations positively, charged atoms or groups of atoms. Radicals are uncharged groups of atoms which occur (not necessarily always filling the same role) throughout a number of compounds and do not normally exist in the free state; when they exist independently and uncharged they are "free radicals"; when charged they become ions. Names of radicals end in -yl. Names of ions are, in general, those of the electropositive or electronegative "constituents" described in the preceding sections; names of cations thus have no characteristic ending; those of anions end in -ide, -ite, -ate. Thus Na^+ is the sodium ion, or more precisely, the sodium cation. Fe^{2+} is the ferrous ion, or iron(II) ion, or ferrum(II) ion (or cation may replace ion). I^- is the iodide ion or iodide anion, so it obviously is not wise to abbreviate the less common I^+ iodine cation.

There are a few special points to be noted, particularly where the I.U.P.A.C. 1957 rules choose between previous alternative usages.

NO^+ is to be called the nitrosyl cation, $NO_2{}^+$ the nitryl cation (not nitroxyl, to avoid confusion with the radical from nitroxylic acid).

Polyatomic cations formed by adding protons to monoatomic anions have the ending -onium: ammonium, phosphonium, arsonium, oxonium (H_3O^+), sulphonium, selenonium, telluronium, iodonium. Substituted derivatives may be formed from them, *e.g.*, hydroxylammonium, tetramethylstibonium, dimethyloxonium $(CH_3)_2OH^+$.

For nitrogen bases other than ammonia and its substitution products the cations are named by changing the final -e to -ium: anilinium, imidazolium, glycinium, *etc.* $N_2H_5^+$ is hydrazinium(1+); $N_2H_6^{2+}$ is hydrazinium(2+). Uronium and thiouronium (from urea and thiourea) are exceptions. Names such as dioxanium and acetonium are formed analogously.

Finally, though H^+ is the proton, and H_3O^+ (a monohydrated proton) is oxonium, the name hydronium is that for a proton with an indefinite degree of hydration, and hydrogen ion can be used when the degree of hydration is of no importance in the particular circumstances.

Radicals having special names are listed in *Table* 3. Thio-, seleno-, *etc.*, prefixes may be used with these, as with acids. The "-yl" principle is noted in the rules as not extensible to other metal–oxygen radicals. In some cases use of Stock numbers extends the range, *e.g.*, UO_2^{2+} uranyl(VI), UO_2^+ uranyl(V); vanadyl(V). vanadyl(IV), and vanadyl(III) all exist.

Table 3. SPECIAL INORGANIC RADICAL NAMES

HO	hydroxyl	S_2O_5	pyrosulphuryl
CO	carbonyl	SeO	seleninyl
NO	nitrosyl	SeO_2	selenonyl
NO_2	nitryl	CrO_2	chromyl
PO	phosphoryl	UO_2	uranyl
VO	vanadyl	PuO_2	plutonyl†
SO	sulphinyl (thionyl*)	ClO	chlorosyl‡
SO_2	sulphonyl (sulphuryl*)	ClO_2	chloryl‡
		ClO_3	perchloryl‡

* For use only with halides.
† Similarly for other actinides.
‡ Similarly for other halogens.

These radicals lead to names such as:

$COCl_2$	carbonyl chloride
PON	phosphoryl nitride
$PSCl_3$	thiophosphoryl chloride
$CrOCl_2$	chromyl chloride
IO_2F	iodyl fluoride
SO_2NH	sulphonyl imide
$VO(SO_4)_2$	vanadyl(IV) sulphate

In such cases the -yl radical is handled as if it were the electropositive part of a name, but no polarity considerations should in fact apply: NOCl is nitrosyl chloride, and $NOClO_4$ is nitrosyl perchlorate independently of views on polarity.

The radical names, then, are convenient for certain groups of compounds, but other, superficially similar compounds are often better named as mixed oxides or oxide salts (see below).

The I.U.P.A.C. 1957 rules use these radicals also for amides, giving $SO_2(NH_2)_2$ sulphonyl diamide and $PO(NH_2)_3$ phosphoryl triamide. As alternatives they give sulphuric diamide and phosphoric triamide. For the partial amides they put forward -amidic acid names (as in the Anglo-American phosphorus rules[6]) and as an alternative the use of co-ordination nomenclature; for example, $NH_2{\cdot}SO_3H$ sulphamidic acid or amidosulphuric acid. Abbreviated names—in the above cases the common sulphamide, phosphamide, and sulphamic acid—are "not recommended". However, the -yl amide names differ noticeably from present organic practice, where amides are a much larger class than in inorganic chemistry; it seems to the present writer better to use either the trivial names or the co-ordination names at present: for example, $SO_2(NH_2)_2$ sulphamide; or, for new compounds, as in dioxodiaminosulphur.

Salts and salt-like compounds

(*a*) *"Acid" salts, i.e., salts containing acid hydrogen.* Names are formed by adding hydrogen, to denote the replaceable hydrogen present, immediately before the name of the anion.

The non-acidic hydrogen present, *e.g.*, in the phosphite ion, is included in the name of the anion and is not explicitly cited (*e.g.*, Na_2PHO_3 sodium phosphite).

Examples:

$NaHCO_3$	sodium hydrogencarbonate
NaH_2PO_4	sodium dihydrogenphosphate
$NaH[PHO_3]$	sodium hydrogenphosphite

That is a direct transcription from the 1957 I.U.P.A.C. rules. The wording does not specify that "hydrogen" is to be joined directly to the anion, but that is done in these and other examples. The citation of acidic hydrogen is classical nomenclature. The non-citation of non-acidic hydrogen is reasonable* (though the present author would write "monosodium" in the last example, to avoid possible misinterpretation). The junction of two words (hydrogen and the anion) which have independent existence, without any form of punctuation, is uncommon in British nomenclature; its nearest relative is the American conjunctive nomenclature in organic chemistry (see p. 40); The Chemical Society has decided to write hydrogen and the anion as separate words.

It is to be noted that names such as bicarbonate and bisulphate are not permitted; nothing similar is anyway possible for polybasic acids; hydrogen has

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* It applies only to trivial names of acids and their anions (*cf. Table* 2, p. 18), and not when the co-ordination principle is applied: *e.g.*, $NaH[PHO_2F_2]$ would be sodium hydrogenhydridodioxodifluorophosphate, the non-acidic hydrogen being cited here as hydrido.

long been cited in such cases in Chemical Society publications (but often not elsewhere). Ions should be similarly named, *e.g.*, hydrogen carbonate ion.

(*b*) *Double salts, etc.* All cations are cited before all anions; cations should be in order of increasing valency (except H^+), and, for cations of the same valency, in order of decreasing atomic number, with polyatomic ions (*e.g.*, NH_4^+) last in their group; anions are to be in the same order as for co-ordination compounds (p. 16). Water considered to be co-ordinately bound to a specific ion is cited as aquo-. Numerical prefixes can be omitted if the valencies are constant or stated. Examples are:

$TlNa(NO_3)_2$	thallium(I) sodium nitrate *or* thallium sodium dinitrate
$NaZn(UO_2)_3(C_2H_3O_2)_9,6H_2O$	sodium zinc triuranyl acetate hexahydrate
$Na_6ClF(SO_4)_2$	(hexa)sodium chloride fluoride bis(sulphate)

In the last example, either one of the numeral prefixes may be omitted. Note, too, the use of bis(sulphate) to avoid confusion with disulphate ($S_2O_7^{2-}$).

(*c*) *"Basic" salts.* These are to be named as double salts with O^{2-} or OH^- anions; names such as hydroxychloride join the constituents together incorrectly and should not be used (in English). The I.U.P.A.C. class names are oxide salts and hydroxide salts, *e.g.*

$Mg(OH)Cl$	magnesium hydroxide chloride
$BiOCl$	bismuth oxide chloride
$Cu_2(OH)_3Cl$	dicopper trihydroxide chloride

(*d*) *Double oxides and hydroxides.* These are named on similar principles.

$FeTiO_3$	iron(II) titanium trioxide
$Cu(CrO_2)_2$	copper(II) chromium(III) oxide

(Copper chromite is considered incorrect for the last example, in view of the results of structural studies on the solid.)

Classical co-ordination compounds

These are the compounds where the oxidation number is exceeded. Most of the principles governing their nomenclature have been explained above. The main features may be recapitulated as follows. The complex may be cationic, neutral, or anionic. Cationic or neutral complexes have no special ending (except -ium for quaternary ions); names of anionic complexes end in -ate. Ligands are cited in the order (*i*) anionic, in a specified sub-order, (*ii*) neutral and cationic ligands, in a specified sub-order. Stock numbers or stoicheiometric proportions or both are cited, as necessary. Cationic and neutral ligands have unaltered names; anionic ligands are given the ending -o.

The following additional principles are to be noted:

(*a*) Water, co-ordinated inside a complex, is cited as aquo-, ammonia as ammine.

(*b*) Hydrocarbon radicals have the usual organic names ending in -yl (not -ylo).

(*c*) CH_3O^-, *etc.*, are called methoxo-, *etc.*

(*d*) HS^- is thiolo-, S^{2-} thio-, and, *e.g.*, $CH_3{\cdot}S^-$ methanethiolato-.

(*e*) When an organic compound which is not normally named as an acid forms a ligand *by loss of a proton*, it is treated as anionic and its name is given the ending -ato. (In other cases it is treated as neutral.)

(*f*) For computation of the oxidation number, NO, NS, CO, and CS are treated as neutral; hydrocarbon radicals are counted as negative (to avoid unusual results).

After these explanations the following examples will, it is hoped, be self-explanatory and sufficiently illustrate the principles:

$[CoN_3(NH_3)_5]SO_4$	azidopentamminecobalt(III) sulphate
$[CoCl(NH_3)_5]Cl_2$	chloropentamminecobalt(III) chloride
$[Cr(H_2O)_6]Cl_3$	hexaquochromium(III) chloride *or* hexaquochromium trichloride
$[Co(NH_2)_2(NH_3)_4]OC_2H_5$	diamidotetramminecobalt(III) ethanolate
$[Ru(HSO_3)_2(NH_3)_4]$	bis(hydrogen sulphito)tetrammineruthenium(II)
$K_2[Cr(O)_2O_2(CN)_2(NH_3)]$	potassium dioxoperoxodicyanoamminechromate(VI)
$Na[BH(OCH_3)_3]$	sodium hydridotrimethoxoborate
$K_2[Fe_2S_2(NO)_4]$	dipotassium dithiotetranitrosyldiferrate
$[CuCl_2(CH_3{\cdot}NH_2)_2]$	dichlorodi(methylamine)copper(II)
$[Pt\ py_4][PtCl_4]$	tetrapyridineplatinum(II) tetrachloroplatinate(II)
$[PtCl_2(H_2N{\cdot}CH_2{\cdot}CH(NH_2){\cdot}CH_2{\cdot}NH_3)]Cl$	dichloro-2,3-diaminopropylammoniumplatinum(II) chloride
$[Ni(C_4H_7O_2N_2)_2]$	bis(dimethylglyoximato)nickel(II)
$[CoCl_2(C_4H_8O_2N_2)]$	dichlorobis(dimethylglyoxime)cobalt(II)
$Na_2[Fe(CN)_5NO]$	disodium pentacyanonitrosylferrate
$HCo(CO)_4$	hydrogen tetracarbonylcobaltate(−1)
$Fe_2(CO)_9$	enneacarbonyldi-iron

$H_2[Fe(CO)_4]$	dihydrogen tetracarbonylferrate
$K[SbCl_5C_6H_5]$	potassium pentachloro(phenyl)antimonate(V)
$K_2[Cu(C_2H)_3]$	potassium triethynylcuprate(I)
$Fe(C_5H_5)_2$	bis(cyclopentadienyl)iron(II)
$[Fe(C_5H_5)_2]Cl$	bis(cyclopentadienyl)iron(III) chloride
$Cr(C_6H_6)_2$	dibenzenechromium

The handling of carbonyl derivatives in the examples will be noted: names such as di-iron enneacarbonyl (with its "irregular" final -yl ending) and iron carbonyl hydride or iron tetracarbonyl dihydride (with its incorrect use of hydride) can well be spared. The last three names show that π-bonding is no bar to the use of the co-ordination nomenclature.

Bridging groups are indicated by μ, as in:

$[(CO)_3Fe(CO)_3Fe(CO)_3]$	tri-μ-carbonylbis(tricarbonyliron)
$[Be_4O(O{\cdot}CO{\cdot}CH_3)_6]$	μ₄-oxo-hexa-μ-acetatotetraberyllium (where the inferior 4 indicates that the oxygen bridges four atoms)

Extended structures are indicated by catena:

$[Cs]_n[\ldots CuCl_2–Cl–CuCl_2–Cl–CuCl_2–Cl \ldots]^{n-}$
caesium catena-μ-chlorodichlorocuprate(II)

Isopolyanions

Numerical prefixes suffice:

$K_2S_2O_7$	potassium disulphate
$Ca_3Mo_7O_{24}$	tricalcium heptamolybdate

Heteropolyanions

Co-ordination principles are applied for naming the polyanion. Here again numerical prefixes (or prefixed numerals in complex cases) are preferred in the

1957 I.U.P.A.C. rules; collecting the numbers of the atoms in parentheses at the end, as in $5Na_2O,12WO_3$ sodium tungstate(10:12:41), becomes impracticable in complex cases. The examples (some are given below) require, however, considerable arithmetical calculation before the formula can be derived from the name.

$Na_6P_2Mo_{18}O_{62}$	hexasodium 18-molybdodiphosphate
$K_3PV_2Mo_{10}O_{39}$	tripotassium decamolybdodivanadophosphate

Addition compounds, including solvates

The ending -ate being reserved exclusively for anions, the 1957 I.U.P.A.C. rules categorically reject the names ammoniate, etherate, *etc.*, but, with reluctant deference to custom, accept hydrate as an alternative. Their method of naming is shown by the following examples:

$CaCl_2,6H_2O$	calcium chloride–6-water (or calcium chloride hexahydrate)
$AlCl_3,4C_2H_5{\cdot}OH$	aluminium chloride–4-ethanol *or* -tetrakisethanol
$8H_2S,46H_2O$	8-hydrogen sulphide–46-water
$8CHCl_3,16H_2S,136H_2O$	8-chloroform–16-hydrogen sulphide–136-water
$CaCl_2,8NH_3$	calcium chloride–8-ammonia
$BF_3,(C_2H_5)_2O$	boron trifluoride–diethyl ether

This is little more than speaking the formula. The alternative seems to be "boron trifluoride-ether complex", *etc.*, and chemists have long mostly written merely "boron trifluoride-ether", so perhaps the I.U.P.A.C. names are (temporarily) acceptable.

Naturally, if part of the adduct is believed to be co-ordinately bound to a specific atom, then that can be expressed in the name, as in:

$FeSO_4,7H_2O$ *or* $[Fe(H_2O)_6]SO_4,H_2O$ iron(II) sulphate heptahydrate *or* hexaquoiron(II) sulphate monohydrate

$AlCl_3,NOCl$ *or* $NO[AlCl_4]$ aluminium chloride–nitrosyl chloride *or* nitrosyl tetrachloroaluminate

REFERENCES

1 See *J. chem. Soc.*, 1940, 1404.

2 *I.U.P.A.C. Comptes rendus of the* 17*th Conference*, 1953, pp. 98–119.

3 *I.U.P.A.C. Nomenclature of Inorganic Chemistry*, 1957, Butterworths, London, 1959.

4 *Cf.* MITCHELL, A. D., *British Chemical Nomenclature*, Arnold, London, 1948, p. 10.

5 *I.U.P.A.C. Comptes rendus of the* 15*th Conference*, 1949, pp. 127–132.

6 See *J. chem. Soc.*, 1952, 5122–5131.

3

ORGANIC: GENERAL

Organic chemical nomenclature is an infuriating subject. Since some three-quarters of a million organic compounds are known and it is a century since Couper and Kekulé explained the fundamental principles of structure, we might expect chemists to define the constitutions and interrelations in an orderly way. Instead, systems of nomenclature pre-dating Kekulé survive; Heilbron's *Dictionary*[1] and Beilstein's *Handbuch*[2] show trivial names in profusion to benumb memory; two major collations of nomenclature in the English language (Mitchell's book[3] and *Chemical Abstracts* Indexes[4]) show bewildering differences; and Stelzner's *Literatur-Register*[5] and the *Ring Index*[6] give different names for about half the cyclic skeletons common to them.

The first international rules (Geneva, 1892) were revised, and substantially altered, by the Commission on the Nomenclature of Organic Chemistry of the International Union of Chemistry in 1930 (Liége). These 1930 rules[7] still form the basis of much correct practice but they are sadly incomplete and in places ambiguous. The Union* began a new revision and great extension in 1947; about half of this work is now complete (1959)[8, 9].

I.U.P.A.C. 1957 nomenclature rules, with any necessary extensions and a few very minor modifications, are accepted by The Chemical Society as the basis of sound practice and have been reprinted by the Society with editorial notes[10].

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* In 1949 the older title "International Union of Pure and Applied Chemistry" (I.U.P.A.C.) was re-assumed.

The remainder of this chapter will deal with general matters; later chapters deal with specific aspects.

CONVENTIONS

These vary from one publishing Society and House to another, linguistic difficulties and personal preferences preventing agreement.

Punctuation

A useful step has been taken by the Chemical Societies of America and Britain in a very recent agreement: commas will be used between numerals referring to multiple identical operations, as in 1,2,6-tribromohexane; colons will be used between groups of numerals for similar but distinct operations, as in 1,2:5,6-di-*O*-isopropylidenesorbitol. (Here the major change is for Great Britain.)

Numerals

In Great Britain numerals should be placed immediately in front of the syllables to which they refer, independently of whether these syllables are prefixes or suffixes. For example, we have 2-chlorohexane, 2,3-dichlorohexane, 3-bromo-2-chlorohexane, hexan-2-ol, hexane-2,3-dione, hex-2-ene, hexa-2,4-diene, hex-2-en-4-yne, hex-2-en-4-yn-1-ol. For radicals British practice varies: for common radicals it is customary to write the numeral in front of the whole stem, as in 2-naphthyl (or β-naphthyl) or 3-chloro-2-pyridyl; in more complex cases it is obviously clearer to place the numeral referring to the radical linkage before the syllable -yl, as in 1,3-oxazin-2-yl; in intermediate cases it is safer, though not essential, to adopt the latter course, as in, *e.g.*, 1-methylimidazol-4-yl. (The position of numerals for suffixes or radicals varies widely from country to country. In America one numeral is placed in front of the stem, as in 2-hexanol or 2-hexene; for several suffixes of the same kind the numerals remain in front, as in 2,3-hexanediol; for suffixes of more than one kind, the numeral for the suffix occurring first in the name remains in front, as in 2-hexen-3-ol or 2-hexen-4-yn-1-ol. This must be remembered when reading *Chemical Abstracts*. Readers of Beilstein's *Handbuch*, however, have to remember that in Germany numerals for suffixes are generally placed after the suffix, and often in parentheses: hexanol(3) or hexanol-3; hexen(2)ol(3). French custom tends to the German practice but often with spaces between parts of the name.)

Group symbols

The Chemical Society uses the following abbreviations for groups; they will be used here, too:

CH_3-	Me
$CH_3\cdot CH_2-$	Et
$CH_3\cdot CH_2\cdot CH_2-$	Pr^n
$(CH_3)_2CH-$	Pr^i
$CH_3\cdot CH_2\cdot CH_2\cdot CH_2-$	Bu^n
$(CH_3)_2CH\cdot CH_2-$	Bu^i
$CH_3\cdot CH_2\cdot CHMe-$	Bu^s
$(CH_3)_3C-$	Bu^t
$CH_3\cdot CO-$	Ac
C_6H_5-	Ph
$C_6H_5\cdot CO-$	Bz (not to be used for benzyl)

Decimal points are written to separate individual single groups, but not when parentheses are involved (see above). (N.B. The American Chemical Society does not use this punctuation, writing simply $CH_3CH_2CH_2-$, *etc.*) The central atom of a group is normally written first (CH_4, CH_3-); this convention reduces the number of decimal points needed ($-CHMe-$; $-NHPh$; $NO_2\cdot C_6H_4\cdot NHMe$).

Italicizing

By a recent Chemical Society decision, prefixes will be italicized if, and only if, (*i*) they define the position of named substituents or (*ii*) they define a stereoisomer. Thus italics, by clause (*i*) continue, for example, to be used for *o*-, *m*-, *p*-, and for element symbols which denote substitution on that element, as in *o*-dichlorobenzene, *N*-methyl-2-naphthylamine, *etc.* By clause (*ii*), italics continue to be used for *cis*-, *trans*-, *syn*-, *etc.* But italics are no longer used in names such as isobutane, isopropyl, t-butyl, for here, though the prefixes define the substance, they do not define *named* substituents. Similarly prefixes which have varied use are not italicized when in particular cases they refer to stereoisomers, as in allocinnamic acid, for here they do not *define* a particular stereoisomer. These new rules involve other frequent changes from previous British practice, notably that cyclo, iso (as in isoquinoline, isocyanide), spiro, neo, pseudo, allo, epi, and several other "general" prefixes will in future be in roman, not italic, type. The new rules differ somewhat from American practice and previous British practice. Italicized prefixes are neglected for capitalizing at the beginning of a paragraph or after a full stop, and also in indexes (*e.g.*, *m*-Xylene, *cis*-Stilbene).

Alphabetical order

In British and American nomenclature, prefixes are arranged in alphabetical order. The atoms and groups are alphabeticized first and the multiplying prefixes are then inserted, as in:

o-bromochlorobenzene
4-ethyl-3-methyldecane
1,1,1-trichloro-3,3-dimethylpentane

A complex radical forms one suffix; it is therefore alphabeticized under its first letter, as in:

1-dimethylamino-3-ethyl-4-methylamino-2-naphthoic acid
4-chloro-1,5-bisdimethylamino-3-ethyl-2-naphthoic acid

For otherwise identical prefixes the one with the lowest locant at the first cited point of difference is given first, as in:

1-(2-ethyl-3-methylpentyl)-8-(2-ethyl-4-methylpentyl)naphthalene

When two words fill identical functions in a three-word name they are alphabeticized, as in:

ethyl methyl ketone
butyl ethyl ether

Italics are neglected in alphabeticizing, as in:

3-*trans*-but-2′-enyl-2-ethylphenol

Elision

The terminal "e" is elided before a vowel of an organic suffix, independently of interruption by a numerical prefix, but not in similar chemical circumstances when the following letter is a consonant: examples are propane → propanone; hexan-2-one; hexane-2,3-dione. Elision is undesirable in organic names in other places: the large number of trivial names offers traps for the unwary (*cf.* tetronic acid).

Hyphens

These are used in British chemical work between two identical letters in chemical names (*e.g.*, tetra-acetate, methyl-lithium), to help reading in such words as co-ordination and un-ionized (not a union). and to separate portions of partial names such as keto-ester, amino-acid. By a long-established custom The Chemical Society uses hyphens also when partial chemical names end in a voiced vowel or "y", *e.g.*, amino-derivative, thia-compound, methoxy-group, but not after a consonant or unvoiced vowel in such places, *e.g.*, methyl derivative, amide group; the reason is probably that, in English, chemical words do not end in vowels. Further, in Chemical Society practice, hyphens are used in composite class names, *e.g.*, keto-acid, chloro-ketones, oxo-steroids.

Parentheses

Parentheses are used when necessary to clarify the limits of an operation but must not be used unnecessarily. In The Chemical Society's practice they are considered unnecessary for names such as 1-2′-chloroethyl-2-naphthol, 1-*p*-aminophenylbutanol, or even *p*-di-2′-chloroethylbenzene; they are used when more than one numeral is included in the substituent name, primes being then unnecessary, as in *N*-(2,4-dinitrophenyl)glycine or 1-(4-amino-2-ethylphenyl)butanol. Parentheses are also used to clarify a few special usages, *e.g.*, to distinguish (phenylthio)acetic acid $PhS{\cdot}CH_2{\cdot}CO_2H$ from phenyl(thioacetic) acid $Ph{\cdot}CH_2{\cdot}COSH$.

Multiplicative numerical prefixes

These are used to qualify a group whose name begins with a (usual) numerical prefix, *e.g.*, bis-2,4-dinitrophenylhydrazone. They may also be used with composite names when the standard prefix would be misleading, *e.g.*, NMe_2 dimethylamino, but $(NHMe)_2$ bismethylamino; however, in the latter type of case di(methylamino) is equally satisfactory, at least in writing.

TECHNICAL TERMS

A few definitions[10] may clarify thought and discussion.

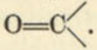
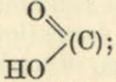
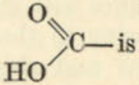
Parent. We think of benzene as the chemical parent of nitrobenzene because the latter is made from the former; and benzene is the parent name of nitrobenzene because the latter is derived from the former by a prescribed variation. However, parent names do not always reflect chemical parentage: ethane is hardly the chemical parent of ethanol, though ethane is the parent name of ethanol. Often there is a chain of parentage—hexane, 3-methylhexane, 3-chloromethylhexane –or multiple parentage—benzanthracene from benzene and anthracene.

Systematic name. A name composed wholly of specially coined or selected syllables: hexane, thiazole.

Trivial name. A name no part of which is used in a systematic sense: xanthophyll, furan.

Semisystematic = semitrivial name. A name of which only a part is used in a systematic sense: meth*ane*, but*ene*, calcifer*ol*. Most names in organic chemistry belong to this class; many are often spoken of loosely and incorrectly as simply "trivial".

Group or radical. A group of atoms common to a number of compounds (as in inorganic chemistry; CH_3, CH_2, OH, NO_2, CO, CO_2H, *etc.*).

Function, functional group. These terms are often misused, perhaps even usually misused. They entered English nomenclature in I.U.P.A.C. rules by translation from the 1930 French version (fonction, fonctionnel) without definition. A functional group is a group of atoms defining the "function" or mode of activity of a compound. An alcohol owes its alcoholic properties to the functional group –OH; here the functional group, hydroxyl, is the same as the chemical group of the same name. However, a ketone owes its ketonic properties to the oxygen atom which is doubly bound (to carbon); the ketonic function is O=(C) (without the carbon), and this is not the same as the ketonic group . Similarly the carboxylic function is due to the group  $\mathrm{(HO)(O{=})(C)}$;  $\mathrm{(HO)(O{=})C}$— is the carboxyl group. In most chemical writing we find "function", "group", and "radical" used interchangeably; but they are not interchangeable; usually group or radical expresses the meaning intended, function being used only to sound more technical or "grander". Incidentally, the division of substituents into "functional" and "non-functional" in the fourth edition and first two supplements of Beilstein's *Handbuch* is also incorrect, or at best a special usage.

THE PRINCIPLES OF ORGANIC NOMENCLATURE

There is a fundamental distinction between the use of trivial and of systematic names: trivial names refer to compounds, systematic names to structures, *i.e.*, structural formulae. Trivial names are independent of structure; they can be, and often are, assigned before the structure is known; and when the structure is known, the one name embraces all dynamic variations due to tautomerism, *etc.* A systematic name, being derived from one formula, cannot, if it is accurately descriptive, apply to a tautomer thereof (though normally it covers changes due to resonance, hyperconjugation, *etc.*). For example, acetoacetic acid is, by modern standards, a trivial (actually semitrivial) name: in the keto-form the substance is β-oxobutyric acid or 3-oxobutanoic acid; in the enolic form it is β-hydroxycrotonic acid or 3-hydroxybut-2-enoic acid.

In a semitrivial name an indication of partial structure is built in (*e.g.*, the alcoholic group in ethanol); it is important that this indication be correct, *e.g.*, that acidic phenols be not *named* acids, and that variations of the trivial name for derivatives be made in accordance with the rules for systematic nomenclature.

Owing to the formation, by covalent linkages, of chains and rings of carbon atoms, alone or with heteroatoms (*i.e.*, atoms other than carbon), the structures of organic compounds differ fundamentally from those of nearly all inorganic compounds. The two nomenclatures therefore use quite different methods. Organic nomenclature has, however, been of slow growth and in its present state no less than eight principles can be distinguished.

(*a*) The basic principle is substitution, the replacement of hydrogen by an atom or group, *e.g.*, of H by Cl (chlorination), by NO_2 (nitration), by Me (methylation), even though this replacement may not be the method of synthesis.

The reverse holds, too: chlorination, for instance, is only replacement of H by Cl; the term must not be used for addition, as in: $Ph\cdot CH:CH_2 + Cl_2 \rightarrow Ph\cdot CHCl\cdot CH_2Cl$, or the reaction $\rangle\!\!-C\cdot OH \rightarrow \rangle\!\!-C\cdot Cl$.

Substitution is indicated by a suffix (ethane, ethanol) or a prefix (benzene, chlorobenzene), the loss of hydrogen not being stated.

(*b*) By substitutive nomenclature one reaches the name 2-naphthylacetic acid for $2\text{-}C_{10}H_7\cdot CH_2\cdot CO_2H$, substitution of the naphthyl radical into acetic acid. *Chemical Abstracts*, however, do not find such names useful for indexing; the parent is acetic acid, and after inversion the index entry would be Acetic acid, 2-naphthyl-; but the compound is more suitably indexed under the larger part, naphthalene, and they

achieve this by juxtaposing the two names naphthalene and acetic acid and preceding them by the positional numeral; they thus obtain 2-naphthaleneacetic acid (for indexing under N), the loss of *two* hydrogen atoms being assumed in this process (just as the loss of *one* is assumed in substitutive names). This is termed "conjunctive nomenclature". It is little used in British works, but must be understood by all chemists who read American books or journals or use *Chemical Abstracts*.

(*c*) What is superficially a mixture of substitutive and conjunctive nomenclature is the (universal) practice with prefixes for bivalent groups, such as –O– oxy, $\rangle C{=}O$ carbonyl, –S– thio. Suppose we wish to treat MeO–CO– as a substituent: we place the radical name methoxy next to the bivalent radical name carbonyl and obtain methoxycarbonyl MeO·CO–, *no* hydrogen being lost in the process; then we can substitute this group into, say, glycine $NH_2\cdot CH_2\cdot CO_2H$, with the usual loss of one hydrogen atom in the process, obtaining *N*-methoxycarbonylglycine $MeO\cdot CO\cdot NH\cdot CH_2\cdot CO_2H$.

(*d*) For some classes old names indicating the function of the compounds survive, *e.g.*, ethyl *alcohol*, diethyl *ether*, ethyl methyl *ketone*, acetic *acid*. The systematist would like these to disappear, for (except for acids) there are alternatives more in keeping with current practice; but such names die hard, if only because the chemist is, after all, interested mainly in the functions, *i.e.*, modes of activity, of his compounds.

(*e*) A few additive reactions survive as a basis for names, *e.g.*, styrene oxide. This is, in fact, one of the few additive names which are worth preserving, for the alternatives 1,2-epoxyethylbenzene and 1-phenyloxiran are less easily recognized by some chemists.

Names such as ergosterol dibromide are also valuable as trivial names preserving the parent component. In general, however, additive nomenclature should be avoided: it forms no part of modern nomenclature. Of course, there is an exception: hydro for addition of hydrogen!

A different kind of additive nomenclature is used when an element increases its valency: *e.g.*, pyridine gives pyridine 1-oxide.

(*f*) Subtraction: Removal of atoms is indicated in a few cases, *e.g.*, dehydro (loss of 2H), anhydro (loss of H_2O), nor (loss of CH_2), de (loss of a specified group; *e.g.*, de-*N*-methyl).

(*g*) Many cyclic skeletons have trivial names; complex cases are handled by joining names of simpler components, by methods described in Chapter 7. There are also systems for such compounds where specific syllables have prescribed meanings for ring structure.

(*h*) A few chemical operations can be designated by specific affixes, *e.g.*, lactone, seco-, -oside.

THE APPROACH TO A NAME

With such an array of possible procedures how does one set about naming a compound of known structure? Occasionally the chemistry under discussion is such that it is best to break the rules: but here let us forget such relatively rare occasions and confine ourselves to the classical methods. Then perhaps the obvious way is to look first for a large recognizable unit—a ring structure or a long chain. Nevertheless, that would be wrong, quite wrong. The first thing to do is to seek out the functional groups: OH, NH_2, CO_2H, SO_3H, *etc.*, and the derived groups OMe, CO_2Et, *etc.*; then, from those present, the "senior", so-called "principal" functional group is found by

means of the list on p. 48. That group, and that alone, is written as suffix, the others become prefixes. The principal functional group sets the whole pattern of nomenclature and numbering, and it is vital to fix that group before anything else is done. Two simple examples show this: $C_{10}H_7{\cdot}C_6H_4{\cdot}CO_2H$ is a naphthylbenzoic acid and not a carboxyphenylnaphthalene, whereas $Ph{\cdot}C_{10}H_6{\cdot}CO_2H$ is a phenylnaphthoic acid; $NH_2{\cdot}CH_2{\cdot}CH_2{\cdot}OH$ is 2-aminoethanol, and not 2-hydroxyethylamine (because OH is senior to NH_2).

For the rest of the name one works back from the principal functional group:

(*A*) Suppose this group is attached to an aliphatic chain. Then (1*a*) choose the most unsaturated straight chain so attached; if there are more than one of equal unsaturation—and this includes the case when there is no unsaturation—choose the longest. Or (1*b*), if there is more than one principal functional group (*e.g.*, more than one CO_2H), choose the straight chain containing the most of them; if there are two such chains, choose the more unsaturated, then the longer, as in (1*a*). Next (2) number the chain, with due regard to unsaturation and substituents, but giving the lowest available number(s) to the principal group(s), as explained later. Lastly, (3) name the chain, add the suffix for the functional group(s), name the other substituents as prefixes, and add them in alphabetical order to complete the name.

Or (*B*) suppose the principal functional group is attached to a ring. Then name the cyclic system, as explained later; number it, giving the lowest available numbers first to the principal functional group and then to the other atoms and groups to be cited; and write down the name as in (*A*3).

(*C*) If the principal functional group is attached to a chain and that in turn to a ring, the British author should treat the cyclic radical as a substituent into the chain. Only if more than one chain is attached to the same cyclic structure will the British author turn to a conjunctive name, as in 1,2-naphthalenediacetic acid.

(*D*) A variant of these procedures is useful for compounds with the symmetrical structural pattern X–Y–X when each of the units X contains the same principal functional group for citation as suffix. Examples are

$$HO_2C{\cdot}CH_2{\cdot}\overset{p}{C_6H_4}{\cdot}CH_2{\cdot}CO_2H$$

and $$H_2N{\cdot}CH_2{\cdot}CH_2{\cdot}O{\cdot}CH_2{\cdot}CH_2{\cdot}NH_2$$

The principal functional groups lead to the endings "-diacetic acid" and "-di(ethylamine)", respectively, in these two cases. The central unit —Y— is cited as the bivalent radical, "*p*-phenylene-" for $-C_6H_4-$ and "oxy-" for O. Locants are added and the full names become *p*-phenylenediacetic acid and 2,2′-oxydi(ethylamine). The parentheses in the latter name serve to remove possible confusion with a derivative of diethylamine.

The 1961 I.U.P.A.C. tentative rules[11] suggest that the principal functional group, *i.e.*, the functional group chosen for description as suffix, be called the "characteristic group"; if adopted finally, this would be valuable as a way to avoid the ambiguities which previous practices have attached to the words "function" and "functional".

There are only a few steps in each case (*A–D*) and, if taken in the right order, they lead simply to the answer. It is surprising how many of the compounds met in ordinary chemistry can be named merely by the above simplified procedures. Of course, it is easier to write "name the ring" than to do it, and tricky problems are sometimes met. The procedures given will be expanded, and some of the problems discussed, in the following pages, but to reach them we must start again systematically at the beginning.

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[2] Beilstein, *Handbuch der Organischen Chemie*, Springer-Verlag, Berlin.

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[5] Stelzner, R., *Literatur-Register der Organischen Chemie*, Springer, Berlin, 1931, Vol. III, 1914–15, pp. 22–24.

[6] Patterson, the late A. M., Capell, L. T., and Walker, D. J., *The Ring Index*, Reinhold, New York, 1959; and two supplements published in 1964.

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[8] *I.U.P.A.C. Comptes rendus of the* 15*th Conference*, 1949, pp. 127–186; 16*th Conference*, 1951, pp. 100–104; 18*th Conference*, 1955, pp. 120–184.

[9] *I.U.P.A.C. Nomenclature of Organic Chemistry*, 1957, Definitive Rules for Section A. Hydrocarbons, Section B. Fundamental Heterocyclic Systems. Butterworths, London, 1958.

[10] For details see "Handbook for Chemical Society Authors", Special Publication No. 14, The Chemical Society, Burlington House, London, W.1.

[11] *I.U.P.A.C. Nomenclature of Organic Chemistry*, 1961. Tentative Rules for Section C. Characteristic Groups Containing Carbon, Hydrogen, Oxygen, Nitrogen, Halogen, Sulfur, Selenium, and/or Tellurium, Butterworths, London, 1962.

4

ORGANIC: THE PRINCIPAL FUNCTIONAL GROUP

A functional group is one which determines the activity of a compound (see p. 38). No clear chemical distinction can be drawn between functional and non-functional groups, but for most purposes of nomenclature a functional group is one whose designation can be added at the end of the complete name of a compound without alteration to that name other than, sometimes, elision of terminal "e".

Table 4 (p. 48) lists some common group names, those in the first portion being functional groups arranged in order of "seniority": a group has priority over one below it in this section of the list for rank as principal functional group and therefore for citation as suffix; as explained on p. 43, there can be only one kind of *principal* functional group in a compound. Groups not on the list rank after their nearest relatives. Clearly, it is not an exhaustive list but it suffices for most purposes.

For example, CO ranks before OH, so that we write 2-hydroxycyclohexanone and not 2-oxocyclohexanol; in the same way OH ranks before NH_2, so that *p*-$HO{\cdot}C_6H_4{\cdot}NH_2$ is *p*-aminophenol and not *p*-hydroxyaniline (an example which shows that the seniority order applies even to semitrivial names). The suffixes and prefixes are used by substitutive nomenclature (with elision of terminal "e"), *i.e.*, the group is considered to replace hydrogen, as in $CH_3{\cdot}CH_3$ ethane → $CH_3{\cdot}CH_2{\cdot}OH$ ethanol, or C_6H_6 benzene → C_6H_5Cl chlorobenzene.

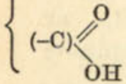
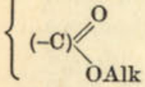
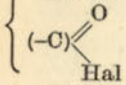
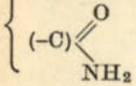
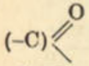
When the carbon atom of a group in *Table* 4 is in parentheses, that atom is not added by the suffix, as when $C_6H_{13}{\cdot}CH_3$ heptane gives $C_6H_{13}{\cdot}CO_2H$ heptanoic acid; when the same group is also listed without parentheses, then the prefix or suffix does add that carbon atom, as in C_9H_9N quinoline → 8-$C_9H_8N{\cdot}CO_2H$ quinoline-8-carboxylic acid, or $(C_3H_7)_2CH_2$ heptane → $(C_3H_7)_2CH{\cdot}CO_2H$ heptane-4-carboxylic acid.

The last column gives the separate word used when the compound is named by the functional method (see paragraph (*d*), p. 41); the preceding word or, for bivalent groups, two words are in radical form, as in ethyl alcohol, ethyl methyl ether, acetyl chloride.

The formation of names by means of *Table* 4 will be familiar from general chemistry, and further examples are unnecessary, but a few special cases should be noted.

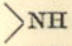
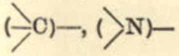
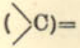
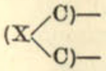
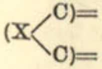
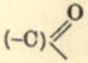
The nomenclature of amines is exceptional. By very long custom radical names may be attached to the ending amine, as in ethylamine; or the prefix amino may be used, particularly if the parent substance is itself basic or is polycyclic, as in 8-aminoquinoline and 1-aminophenanthrene; but it is equally correct to add amine to the parent name, as indicated in *Table* 4, giving names such as phenanthren-1-amine, quinolin-8-amine, or even ethanamine. The last practice is generally reserved for more complex cases and is much more common in America than in Europe. The same alternatives exist for ammonium salts. Secondary and tertiary amines are treated as substitution products of the most complex constituent primary amine, with *N*- prefixes when substitution elsewhere might be reasonable, as in triethylamine, dimethylethylamine, *NN*-dimethylnaphthylamine. Substituted amides, *i.e.*, $R{\cdot}CO{\cdot}NR'R''$, are named as

Table 4. SOME COMMON GROUPS

Group	*Suffix*	*Prefix*	*Separate word*
	A. Functional groups		
N^V	ammonium *		
$-CO_2H$	carboxylic acid	carboxy	
	oic acid		
$-CO{\cdot}OAlk$	alkyl . . . carboxylate	alkoxycarbonyl	
	alkyl . . . oate		
$-SO_3H$	sulphonic acid	sulpho	
$-SO_2H$	sulphinic acid	sulphino	
$-S{\cdot}OH$	sulphenic acid		
$-CO{\cdot}Hal$	carbonyl halide	halogenocarbonyl	
	oyl halide		
$-CO{\cdot}NH_2$	carboxamide	carbamoyl	
	amide		
$-CHO$	carboxaldehyde *or* aldehyde	formyl	
	al, one	oxo	(aldehyde) ketone
$-CN$	carbonitrile	cyano	cyanide
$(-C){\equiv}N$	onitrile		
$-OH$ (alcoholic)	ol	hydroxy	alcohol
$-OH$ (phenolic)	ol	hydroxy	
$-SH$	thiol	mercapto	
$-O-$		epoxy	
$-O{\cdot}OH$		hydroperoxy	hydroperoxide
$-O{\cdot}O-$		peroxy	peroxide

* See text.

Table 4 (*continued*)

Group	*Suffix*	*Prefix*	*Separate word*
	A. Functional groups (*contd.*)		
NH_2	amine *	amino	
NH(Acyl)	amide	amido	
	imine	imino	
$-OAlk$		alkyloxy †	alkyl ether
$-SAlk$		alkylthio	alkyl sulphide
$-SO-$		sulphinyl	sulphoxide
$-SO_2-$		sulphonyl	sulphone
	B. Non-functional groups		
H (added)		hydro	
Halogen		halogeno	halide
$-NO$		nitroso	
$-NO_2$		nitro	
$-N_2O-$		azoxy	
	C. Groups replacing -ane		
$(C){=}(C)$	ene		
$(C){\equiv}(C)$	yne		
		yl ‡	
		idene	
$(-C){\equiv}$		idyne	
		ylene	
		diylidene	
		oyl	

* See text.

† Methoxy to butoxy are used in abbreviated form.

‡ Except morpholino and piperidino.

derivatives of the amide or as amido-derivatives of the parent compound, the more complex constituent being chosen as parent, *e.g.*, *NN*-dimethylbenzamide but 8-acetamidophenanthrene (but the Americans write 8-acetylaminophenanthrene). For salts of amines, and quaternary compounds, see p. 79.

Aldehydes and nitriles may also be named as such when the corresponding acid has a trivial name, *e.g.*, acetaldehyde, benzonitrile.

Whereas ethers of monohydric alcohols or phenols are denoted by alkoxy-, aryloxy-, *etc.*, prefixes or as the -yl -yl ether (with the radical prefixes in alphabetical order), those from polyhydric alcohols and phenols are handled differently. Either the monohydric component is written first, with unchanged -ol ending, as in glycerol 1-ethyl ether, glucose 2,3,6-trimethyl ether; or the ether groups are added by means of *O*- prefixes, as in 2,3,6-tri-*O*-methylglucose, 1-*O*-ethylpyrogallol. The same alternatives exist for esters of polyhydric alcohols.

When there is a choice, unsaturation (-ene, -yne) is denoted rather than hydrogenation (hydro-); for example, cyclohexadiene and not dihydrobenzene.

N.B.

This chapter has dealt with systematic nomenclature; it is not to be taken as excluding the many trivial names to be found in standard books; but it is wise, and good practice, to avoid the less common trivial names except for a purely specialist audience.

5

ORGANIC: NUMBERING

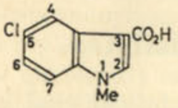
The principles of numbering (enumeration) used for compounds and for radicals are the same, with one exception, namely: for compounds the lowest available numbers are assigned to the principal functional group or groups; for radicals they are assigned to the "free" valency or valencies, and the principal functional groups are here treated merely as ordinary prefixes.

The 1932 international rules[1] on the subject state that for aliphatic compounds lowest numbers are assigned successively, so far as applicable and until a final decision is reached, to (1) the principal function, (2) double bonds, (3) triple bonds, (4) atoms or radicals designated by prefixes, (5) prefixes in order of citation (in Great Britain and America, alphabetical). These rules are applied also so far as possible to all compounds, not merely aliphatic ones.

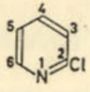
The simplest case is when the numbering of the parent compound is entirely fixed in advance, as occurs with many cyclic compounds (see following chapter). Substituents in, say, indole can have only one number each; compound (I) must be 5-chloro-1-methylindole-3-carboxylic acid.

Next there is the simple case of one group (which need not be a principal function) in a compound such as (II), (III), (IV), or (V) which can be numbered in either of two ways: the lower numbers are as shown and are to be used.

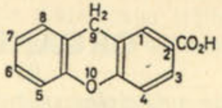
In completely free cases, *e.g.*, (VI), the principal function begins the numbering. If there is more than one functional group, the presence of the second may decide the numbering, either wholly as in (VII), or



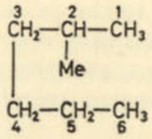
(I)



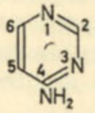
(II)



(III)

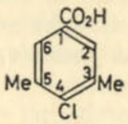


(IV)

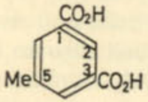


(V)

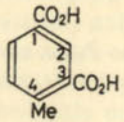
partly as in (VIII) where the methyl group decides which carboxyl group shall have number 1 and which number 3.



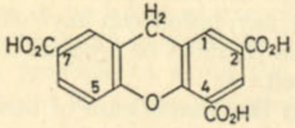
(VI)



(VII)



(VIII)

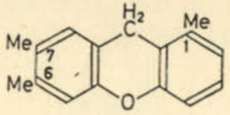


(IX)

CO_2H = 2,4,7- (not 2,5,7-)

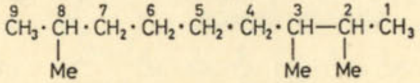
At this stage we need to define "lowest numbers": it is the set of numbers out of a series of sets which contains the lowest number at the first point of

difference. This leads to decisions as shown in cases (IX)–(XIII).



(X)

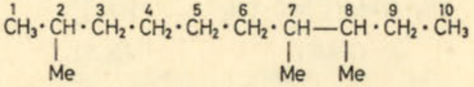
Me = 1,6,7- (not 2,3,8-) (although 1 + 6 + 7 = 14, and 2 + 3 + 8 = 13 only*)



$$\overset{9}{\mathrm{CH_3}}\cdot\overset{8}{\underset{\mathrm{Me}}{\mathrm{CH}}}\cdot\overset{7}{\mathrm{CH_2}}\cdot\overset{6}{\mathrm{CH_2}}\cdot\overset{5}{\mathrm{CH_2}}\cdot\overset{4}{\mathrm{CH_2}}\cdot\overset{3}{\underset{\mathrm{Me}}{\mathrm{CH}}}-\overset{2}{\underset{\mathrm{Me}}{\mathrm{CH}}}\cdot\overset{1}{\mathrm{CH_3}}$$

(XI)

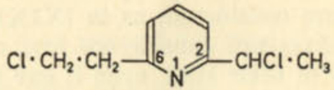
Me = 2,3,8- (not 2,7,8-)



$$\overset{1}{\mathrm{CH_3}}\cdot\overset{2}{\underset{\mathrm{Me}}{\mathrm{CH}}}\cdot\overset{3}{\mathrm{CH_2}}\cdot\overset{4}{\mathrm{CH_2}}\cdot\overset{5}{\mathrm{CH_2}}\cdot\overset{6}{\mathrm{CH_2}}\cdot\overset{7}{\underset{\mathrm{Me}}{\mathrm{CH}}}-\overset{8}{\underset{\mathrm{Me}}{\mathrm{CH}}}\cdot\overset{9}{\mathrm{CH_2}}\cdot\overset{10}{\mathrm{CH_3}}$$

(XII)

Me = 2,7,8- (not 3,4,9-) (although 2 + 7 + 8 = 17, and 3 + 4 + 9 = 16 only*)



(XIII)

1-Chloroethyl precedes 2-chloroethyl

We can now return to the international sequence. (1) The principal functional group decides in cases such as (XIV) and (XV). (2) If there is no functional group, a double bond cited as -ene decides, as in

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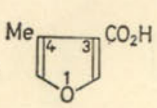
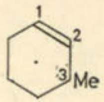
* There has been a belief in some quarters that the total of numbers must be the smallest possible: that is erroneous.

(XVI) and (XVII); also it can make the second choice if the functional group is not decisive, as in (XVIII).

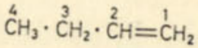


(XIV)

(XV)

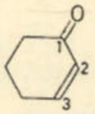


(XVI)

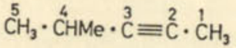


$\overset{4}{C}H_3\cdot\overset{3}{C}H_2\cdot\overset{2}{C}H{=}\overset{1}{C}H_2$

(XVII)

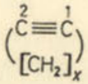


(XVIII)



$\overset{5}{C}H_3\cdot\overset{4}{C}HMe\cdot\overset{3}{C}{\equiv}\overset{2}{C}\cdot\overset{1}{C}H_3$

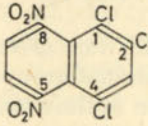
(XIX)



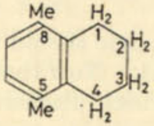
(XX)

Note, however, that unsaturation not cited as -ene is not relevant here: hydro- prefixes are treated in the same way as any other prefix (see below). (3) If there is no principal functional group or -ene double bond, triple bonds are considered, as in (XIX) and (XX). (4) Next, prefixes are considered, first all together, independently of their kind, even if one or more is a functional group (but not the principal functional group), and they include hydro-. Examples are (XXI; 1,2,4,5,8-, not 1,4,5,6,8-), (XXII; 1,2,3,4-tetrahydro), and (XXIII; 1,2,5,8-, not 1,4,5,6-). (5) All other things being equal, the lower number goes to the prefix first cited in the name, as in (XXIV; bromo before chloro), (XXV; ethyl before methyl), (XXVI; dimethylamino before methyl), and (XXVII; tetrahydro before tetramethyl).

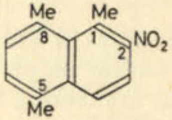
That completes the general rules. Problems, largely theoretical, arising from severe ramification of aliphatic chains are considered in the I.U.P.A.C. 1957 rules[2] but need not be discussed here.



(XXI)

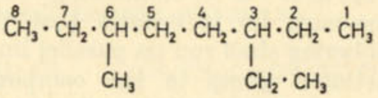


(XXII)



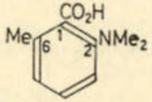
(XXIII)

(XXIV)

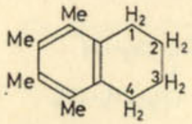


$\overset{8}{C}H_3\cdot\overset{7}{C}H_2\cdot\underset{CH_3}{\overset{6}{C}H}\cdot\overset{5}{C}H_2\cdot\overset{4}{C}H_2\cdot\underset{CH_2\cdot CH_3}{\overset{3}{C}H}\cdot\overset{2}{C}H_2\cdot\overset{1}{C}H_3$

(XXV)



(XXVI)



(XXVII)

REFERENCES

[1] See *J. chem. Soc.*, 1952, 5076.

[2] *I.U.P.A.C. Nomenclature of Organic Chemistry*, 1957. Butterworths, London, 1958.

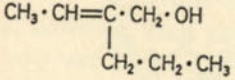
6

ORGANIC: BUILDING A NAME

The ways in which a name should be built were given in outline on pp. 42–44. Now that functional groups and numbering have been discussed, the outline can be filled in.

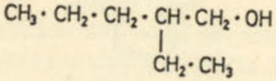
The starting point remains the principal functional group, as it was for numbering. This identity is very important, for it ensures that the name and the numbering shall run on parallel lines. (If there is no functional group in the compound, the name is approached simply as described in the next chapter for skeletal types, and prefixes are added later.)

For aliphatic compounds the complete chain is the parent to which the suffix denoting the principal functional group is added, as in hexan-2-ol. If there is a choice of chains, priority is given to the most unsaturated, as in 2-propylbut-2-en-1-ol (I), even though this may not be the longest. (Double bonds have preference over triple bonds.) If there is a choice between chains of equal degree of hydrogenation, then, of course, the longest chain is chosen, as in 2-ethylpentan-1-ol (II), even though as a result the related compounds (I) and (II) are then named from different parent hydrocarbons.



$$CH_3\cdot CH{=}\underset{\substack{|\\ CH_2\cdot CH_2\cdot CH_3}}{C}\cdot CH_2\cdot OH$$

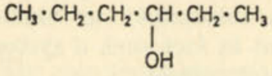
(I)



$$CH_3\cdot CH_2\cdot CH_2\cdot \underset{\substack{|\\ CH_2\cdot CH_3}}{CH}\cdot CH_2\cdot OH$$

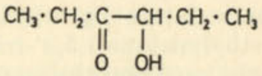
(II)

The principal functional group is the group highest on the list on p. 48. All others, including hydro-,* are given as prefixes, all in alphabetical order. This division into suffix and prefixes can cause chemically unwelcome changes in name or numbering or both: for instance, compound (III) is hexan-3-ol, but (IV) is 4-hydroxyhexan-3-one. The same sort of change can, however, result from shift of a double bond: (V) is 2-ethylhex-1-ene, but (VI) is 5-methylhept-2-ene. The fact is that names are founded on structures, not on chemical relations between two substances; the reason, of course, is that it is often easy to find relationship to more than one other substance so that choice of a name would become ambiguous.



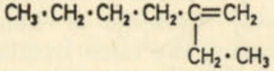
$$CH_3\cdot CH_2\cdot CH_2\cdot \underset{\substack{|\\ OH}}{CH}\cdot CH_2\cdot CH_3$$

(III)



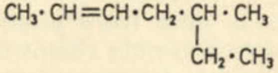
$$CH_3\cdot CH_2\cdot \underset{\substack{\|\\ O}}{C}-\underset{\substack{|\\ OH}}{CH}\cdot CH_2\cdot CH_3$$

(IV)



$$CH_3\cdot CH_2\cdot CH_2\cdot CH_2\cdot \underset{\substack{|\\ CH_2\cdot CH_3}}{C}{=}CH_2$$

(V)



$$CH_3\cdot CH{=}CH\cdot CH_2\cdot \underset{\substack{|\\ CH_2\cdot CH_3}}{CH}\cdot CH_3$$

(VI)

There is no difficulty in citing multiple groups of one kind attached to a single chain or ring system; hexane-3,4-diol and benzene-1,2,3,4-tetracarboxylic acid admit no argument. With branched chains further rules come into play. Substance (VII) must be named so that both functional groups can become suffixes to the principal chain: it is 2-butylpentane-1,4-diol and not 2-2′-hydroxypropylhexan-1-ol, even though this involves a hexane chain and the correct name involves only a pentane chain.

The principle of the preceding paragraph is often spoken of as "treating like things alike". In general

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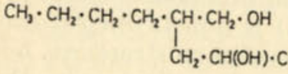
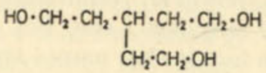
* At least in English and American nomenclature.

that is indeed a good thing to do; but it cannot be made into a guiding light for nomenclature, for there is often argument about degrees of "likeness", and in any case the principle itself must often be discarded. Consider, for example, the simple triol (VIII). Here the name must be based on a pentane chain containing two hydroxyl groups, leaving the third hydroxyl group in a side chain: the correct name is 3-2′-hydroxyethylpentane-1,5-diol. Now there could be a system of nomenclature by which this substance was named 2-ethylpentane-1,5,2′-triol, but in fact such a system is not used and this name is not correct.



$$\mathrm{CH_3{\cdot}CH_2{\cdot}CH_2{\cdot}CH_2{\cdot}\underset{\substack{|\\ CH_2{\cdot}CH(OH){\cdot}CH_3}}{CH}{\cdot}CH_2{\cdot}OH}$$

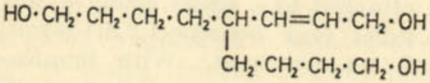
(VII)



$$\mathrm{HO{\cdot}CH_2{\cdot}CH_2{\cdot}\underset{\substack{|\\ CH_2{\cdot}CH_2{\cdot}OH}}{CH}{\cdot}CH_2{\cdot}CH_2{\cdot}OH}$$

(VIII)

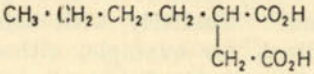
Symmetrical compounds, such as (VIII), are, however, relatively rare. More commonly, branched chains offer more alternatives. Consider a choice between various chains containing the same number of identical groups. As when there was only one functional group, the additional rule favouring unsaturation requires that compound (IX) be named 4-4′-hydroxybutyloct-2-ene-1,8-diol, even though selection of the two saturated branches would give a nonane derivative. When there is no difference in degree of saturation the longer chain would be chosen, and the saturated analogue of the octene (IX) would be 5-3′-hydroxypropylnonane-1,9-diol.



$$\mathrm{HO{\cdot}CH_2{\cdot}CH_2{\cdot}CH_2{\cdot}CH_2{\cdot}\underset{\substack{|\\ CH_2{\cdot}CH_2{\cdot}CH_2{\cdot}CH_2{\cdot}OH}}{CH}{\cdot}CH{=}CH{\cdot}CH_2{\cdot}OH}$$

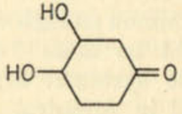
(IX)

There are occasions when further choices are needed for highly branched chains, but they become too theoretical to need discussion here. However, before passing on, let us note that the acid (X) can be called butylsuccinic acid or 2-butylbutane-1,4-dioic acid; whether the trivial succinic or the systematic butanedioic is used, the same principles are applied, leading here to the C_4 chain, not the C_6 chain, as the basis of the name.



$$\mathrm{CH_3{\cdot}CH_2{\cdot}CH_2{\cdot}CH_2{\cdot}\underset{\substack{|\\ CH_2{\cdot}CO_2H}}{CH}{\cdot}CO_2H}$$

(X)



(XI)

The rule about seniority of functional groups, in the order of the list on p. 48, is independent of the relative numbers of the various groups. The compound (XI) is 3,4-dihydroxycyclohexanone, and not 4-oxocyclohexane-1,2-diol: this is in line with the numbering rules (Chapter 5) which give the lowest available number to the principal functional group even though the sequence 1,2,4 is "lower" than 1,3,4. There are many and varied types of problem in which this consideration arises: but the answer is always the same, so further elaboration is unnecessary.

The procedures discussed above are applicable equally when the functional groups are attached directly to cyclic systems. With the more complex ring systems, derivation of the full name is, in fact, usually simpler (once the cyclic parent has been named) because the numbering is at least partly fixed. With simpler ring systems, and particularly the aromatic ones, the systematic procedures become more troublesome, partly from older custom and partly because there is here a very large number of trivial names which should reasonably be carried over to the derivatives.

A systematic name such as naphthalene-2,3-dicarboxylic acid appears perfectly reasonable; but naphthalene-2,3-diol, although correct, may appear strange, at least to older chemists, who would be more at home with 2,3-dihydroxynaphthalene. There are trivial names (which are always used) for many hydroxybenzene derivatives, but hexahydroxybenzene is common enough when the systematic benzenehexaol would be more "correct". Similarly with heterocyclic systems: 2-pyridinol, for example, although usual in America, might in Great Britain be more familiar as 2-hydroxypyridine; pyridinol can be considered correct because the hydroxyl function is senior to amine; yet -ine may be considered as a suffix (a vexed question) and there should be only one suffix; there seems to be no certain criterion for such cases. There is, however, unanimity about the names such as the semitrivial picolinic acid or the systematic quinoline-8-carboxylic acid, where the acid suffix is regularly appended to the -ine ending, so that probably the American argument in favour of pyridinol is the more reasonable.

Special difficulties appear, at least superficially, with amino-derivatives of cyclic compounds. Ethylamine, for example, is almost universal rather than the systematic ethanamine. The semitrivial aniline, toluidine, naphthylamine, *etc.*, are equally familiar, so that even naphthalenediamine may appear strange to many who would prefer naphthylenediamine. Consequently, amines from more complex hydrocarbons are very often named on the pattern of 2-aminophenanthrene or tetra-aminobenzene rather than of phenanthren-2-amine or benzenetetra-amine

which are systematically more correct. More involved are arguments about amino-derivatives of *N*-heterocyclic compounds whose names end in -ine; if the -ine in, say, quinoline is an amine suffix then 2-aminoquinoline appears preferable to quinolin-2-amine because two amine groups should not be denoted by two different suffixes; yet the discussion in the preceding paragraph leaves quinolinamine as perhaps systematically preferable.

With compounds containing both chains and rings the position is simple when the principal functional groups are directly attached either all to the chain or all to the ring system. These groups decide the name parent, *e.g.*, 3-phenylpropan-1-ol but *m*-propylphenol. (However, see pp. 40 and 77 for conjunctive nomenclature.) Nevertheless, when there are principal functional groups attached both to the chain and to the ring system they cannot all be treated as suffixes: the ring system or the chain must be chosen as parent, and the choice will usually fall on that part which is the more complex or the more important chemically, though these criteria are both matters of opinion; sometimes, too, the choice would be the same if made on the number of functional groups in each part. Few would, in fact, quarrel with names such as 8-*p*-hydroxyphenyloctatrien-1-ol or 1-*p*-hydroxyphenylglucose. But it will probably depend on the chemistry under discussion whether a name such as 3-*p*-hydroxyphenylpropan-1-ol or *p*-3-hydroxypropylphenol is chosen.

The previous chapter ended with a warning that systematic names need not displace trivial names in common use. Now we must admit categorically that the systematic approach to a name, as described above, is not always satisfactory. This can be best illustrated by a brief consideration of ketones. The suffix -one and the prefix oxo- are the standard systematic usage. They are in general use when oxygen is doubly bound to a ring-carbon atom, as in cyclohexanone or cholestanone. They are widely used in the aliphatic series, as in 2-hexanone, though here the "ketone" alternatives (butyl methyl ketone, *etc.*) are equally convenient and cannot be regarded as incorrect. But for diaryl ketones, names of the latter type (di-2-naphthyl ketone) are commonest usage, in place of the systematic diarylmethanone which might hardly be understood. For mixed alkyl aryl ketones a third method, also covered in the table on p. 48, is employed: to emphasize the larger aryl component these ketones will generally be named as acyl derivatives, for instance, 1-acetylphenanthrene; yet when two aryl components are present the best approach is to use a name such as 1,4-di-2′-naphthylpentan-3-one, *i.e.*, to revert to the oxo-, -one principle. On the other hand, alkyl phenyl ketones are generally assigned abbreviated names ending in -phenone, such as $Me{\cdot}COPh$ acetophenone, $CH_2{:}CH{\cdot}COPh$ acrylophenone (also $COPh_2$ benzophenone); this is in itself satisfactory; it has been extended fairly frequently to the naphthalene series (2-propionaphthone); it is occasionally extended still further, but this can lead to obvious trouble, as when 1-acetylpyrene becomes 1-acetopyrone (presumably a pyrone derivative) or 1-acetopyrenone (where the -one ending should denote =O attached directly to a ring-carbon atom), and it seems clearly simplest to confine the acetoarone type of name to the benzene series. There is, too, the usual crop of trivial names (benzoin, benzil, chalcone, and many more). Finally, to come full circle back to our first use of -one and oxo-, in cyclic compounds: even this has led to trouble in the heterocyclic series, as will be illustrated in Chapter 8.

It will be clear, then, how the building of a name is not always simply a following of rules. Though in a truly surprisingly high proportion of cases the rules and common trivial names suffice, and though, let it be emphasized again, rules should not be broken without good cause, yet chemistry must not be forgotten. The versatility of organic nomenclature in fact arises from the reasonable wish to express chemical relations in a name; and in this too the difficulties originate, as when multiple chemical relations lead to conflicting types of name or when a specialized usage is extended beyond its appropriate field; then it is wise to revert to the systematic types, which thus remain the backbone of nomenclature. It is essential to appreciate both the uses and the limitations of systematics before indulging in excursions from it.

7

ORGANIC: SKELETAL TYPES

ALKANES AND CYCLOALKANES

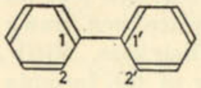
Standard nomenclature is well known, but it may be noted that (*a*) iso- (to denote terminal $CHMe_2$) is restricted to C_3–C_6, t- (tertiary) to C_4 and C_5, and s- (secondary) to C_4[*], (*b*) such modified names may never be used for substituted derivatives of the compounds or radicals, *e.g.*, $CHMe_2{\cdot}CHCl$– is 1-chloro-2-methylpropyl, and (*c*) the free valency of radicals always has number 1, *e.g.*, Pr^n_2CH– is 1-propylbutyl and not 4-heptyl.

BENZENE DERIVATIVES

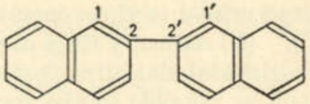
The I.U.P.A.C. 1957 rules[1] follow general custom. Two common misconceptions may be noted. It is no longer customary in Europe to assign lowest numbers to methyl substituents of simple benzene derivatives: the standard rules (see Chapter 5) are applied. There is no such radical as cresyl (from cresol): it is tolyl (*pace* tricresyl phosphate).

BI-COMPOUNDS

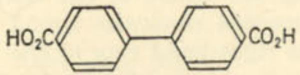
Bi- has long been American usage to denote direct union of two rings, *cf.* (I) and (II), which in Europe were usually called diphenyl and 2,2′-dinaphthyl. The I.U.P.A.C. 1957 rules adopt bi-, and this prefix, useful because it is exclusive and unique for "doubled radicals" (except for bicyclo, see below), has been accepted by The Chemical Society. The I.U.P.A.C. rules, however, permit doubling of either the radical (binaphthyl; II) or the molecule (binaphthalene; II), the bi in the latter cases carrying the implication of loss of two hydrogen atoms as in conjunctive nomenclature (p. 41). The Americans will retain the latter usage (except for biphenyl); The Chemical Society has decided to retain the "doubled radical" names for use with the prefix bi, as in binaphthyl. Numbering is as shown, the points of union having lowest available numbers. The "bi" nomenclature is reserved for unsubstituted compounds, in the sense that only parent compounds may be "doubled"; *e.g.*, compound (III) is biphenyl-4,4-dicarboxylic acid, not *pp′*-bibenzoic acid, as recently in America. Ter, quater, *etc.*, are used for larger ring assemblies, always with the name of the molecule (*e.g.*, ternaphthalene, quaterpyridine), but terphenyl, quaterphenyl, *etc.*, are retained as exceptions owing to long usage: unprimed numbers are assigned to one of the terminal units, the nearest neighbour unit has singly primed and the next doubly primed numbers, and so on; points of union have the



(I)



(II)



(III)

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[*] I.U.P.A.C. rules give *sec*- and *tert*-, but by a recent decision the Chemical Society has adopted s- and t-.

lowest numbers possible, *e.g.*, 2,1′:5′,2″-ternaphthalene.

POLYCYCLIC HYDROCARBONS

(1) Very many trivial names are in use. The I.U.P.A.C. 1957 rules list thirty-five (which supersede any alternatives); only these may be used for fusion names. Except for the long-established anthracene and phenanthrene, these compounds are there numbered by the *Chemical Abstracts* (*Ring Index*) system. The I.U.P.A.C. rules should be consulted for details but in outline the method is as follows.

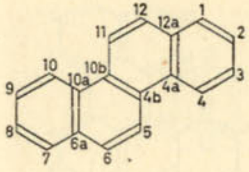
(*i*) Whenever possible, rings are drawn with two sides vertical (a three-membered ring with one vertical). (*ii*) As many rings as possible are then drawn in a horizontal line, irrespective of their size. (*iii*) As much as possible of the remainder of the formula is arranged in the top right quadrant, and as little as possible in the bottom left quadrant (the middle of the first row being the centre of the circle). (*iv*) *Then*, numbering proceeds clockwise round the periphery, starting in the right-hand ring of the top row at the first carbon atom not engaged in ring fusion. Atoms engaged in ring fusion (*i.e.*, at the "valley" positions) receive roman letters a, b, *etc.*, after the numerals of the preceding atom. (Subsidiary rules legislate for less common points.)

Examples are chrysene (IV) and rubicene (V).

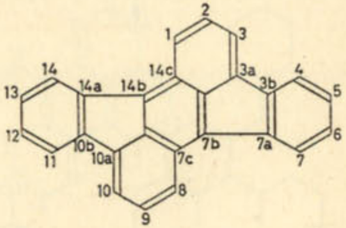
Some cyclic skeletons require a CH_2 component; these components are to be indicated by *H* preceded by a numeral, except when in common compounds such as indene or fluorene its position can be assumed to be the normal one. Thus 3*H*-fluorene is (VI). (This is an improvement on the practice of the first edition of the *Ring Index* and will be adopted in the second edition.)

(2) Polycyclic hydrocarbons not in the I.U.P.A.C. list are named by fusion, for which also the I.U.P.A.C. 1957 rules give the *Chemical Abstracts* (*Ring Index*) system. So many cases are to be covered that again the rules need consultation for complex cases, but the following is an outline of first principles.

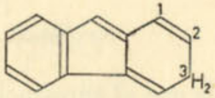
(*a*) The largest possible unit with a trivial name in the list is chosen as base component, and its faces are lettered *a* (italic) for face 1-2, and then *b*, *c*, *etc.*, consecutively around the periphery, as in (VII). The



(IV)

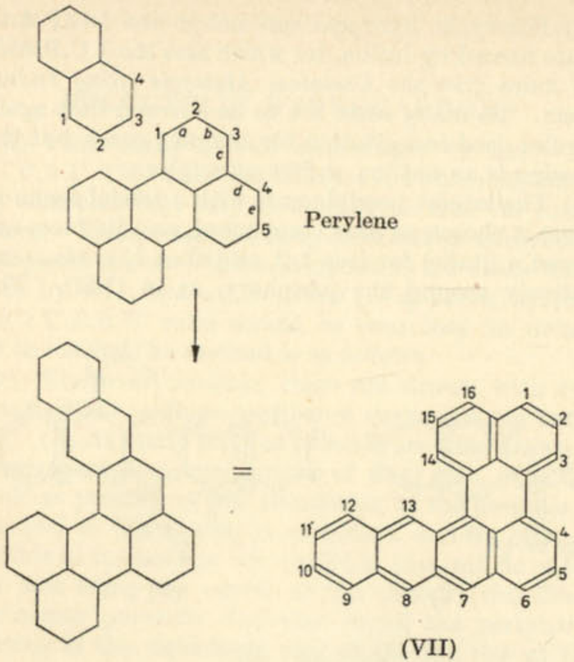


(V)



(VI)

complete name is then built up with an "o" affix and square brackets as shown; the lowest available numbers (independently of substituents) are used for the fusion positions; and the numerals in the brackets must be in an order to correspond with 1,2 for face *a*, *etc.* The formula is then re-orientated, if necessary, to accord with rules (*i*)–(*iii*) above and *re-numbered* in accord with rule (*iv*), as shown in formula (VII) overleaf.



(VII)
Naphtho[2,3-*a*]perylene

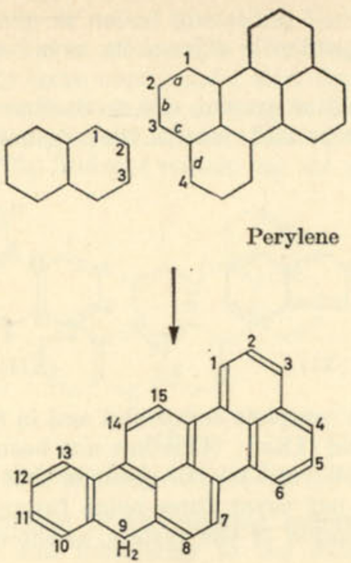
(*b*) Case (VIII) is one of three-point fusion.

(*c*) Designation is simpler for benzo-derivatives such as (IX) and (X).

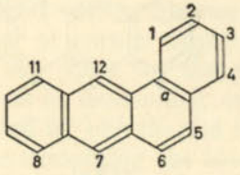
(*d*) Abbreviated names are used for the prefixes benzo, naphtho, anthra (N.B. -a), phenanthro, acenaphtho, and perylo, but not for others.

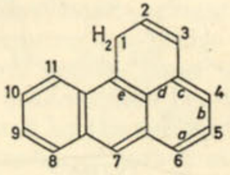
(*e*) The final name applies to the compound with the maximum number of non-cumulative double bonds; thus in indeno[1,2-*a*]indene (XI) the characteristic CH_2 of indene has disappeared.

(*f*) Reduction products are normally indicated by hydro-prefixes (perhydro for complete reduction), but



(VIII)
9*H*-Naphtho[1,2,3-*cd*]perylene





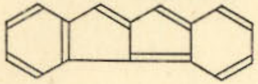
(IX)
Benz[*a*]anthracene

(X)
1*H*-Benz[*de*]anthracene

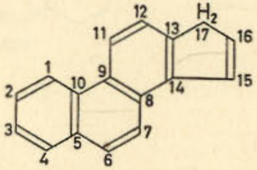
terminal cycloalkene rings may be named by prefixes cyclopenta, cyclo-octa, *etc.*, as in 17*H*-cyclopenta[*a*]phenanthrene (XII). (Incidentally this is treated exceptionally for numbering, receiving the standard steroid treatment as shown.)

(*g*) The "o" indicating fusion is elided before a vowel, independently of brackets, as in benz[*a*]anthracene (IX).

An alternative system, due to Stelzner[2] and much used in Europe still, retains the original numbering,

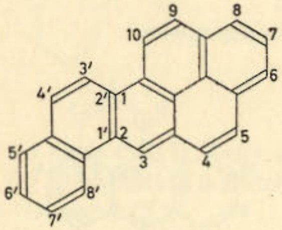


(XI)

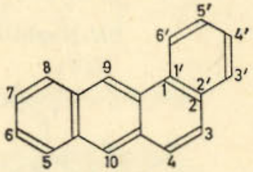


(XII)

both for the complete compound and in the name, as in (VIIa) and (IXa). This has not been adopted in the I.U.P.A.C. rules on the grounds that the original system did not cover three-point fusion, as in case (VIII); extension of the system, as shown in (VIIIa)



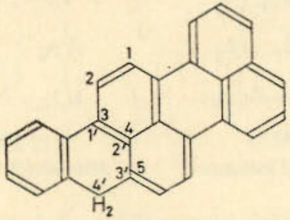
(VIIa)
Naphtho(2′,1′-1,2)pyrene



(IXa)
1,2-Benzanthracene

has, however, been used in The Chemical Society's publications.

Both systems will doubtless continue in use for some time, at least in Europe. The *Chemical Abstracts* system has the advantages that it is more adaptable in complex cases, particularly for reduction products and in the heterocyclic series, that it has been worked out in detail to cover all except a trifling number of exceptionally large compounds, that the ***Ring Index*** on which it is based is the only up-to-date catalogue of all known ring systems, and that it has I.U.P.A.C. approval. The Stelzner system has the advantage of

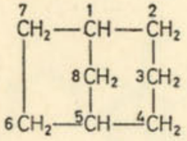


(VIIIa)
4′*H*-Naphtho(1′,2′,3′-3,4,5)perylene

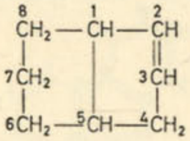
easier recognition of the original numbering of the components and familiarity to the older European chemists.

(3) For naming bridged rings two methods are available. One, the bicyclo-method[3], is particularly suited for highly hydrogenated systems. Count the number of carbon atoms separating one bridge end from the other by the various routes, place these numbers in descending order inside square brackets, preceded by bicyclo and followed by the name of the alkane containing the total number of carbon atoms (now including the bridge atoms), as in (XIII) and (XIV). Numbering starts at one bridge end, goes to the other bridge end by the longest route, continues by the next longest route back to the first bridge end, and finally goes by the last (shortest) path to the second bridge end. Extension of this method to tricyclo-compounds is explained in the I.U.P.A.C. rules; it is complex.

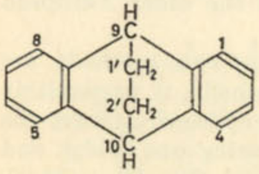
The other method is particularly suitable for bridges across aromatic systems (*e.g.*, Diels–Alder products). It has two variants. In one the bridge is treated as substitution by an arylene *radical* (which retains its own numbering), *cf.* (XV). In the other, by a variation of conjunctive nomenclature (*cf.* p. 41), the name of the bridging *hydrocarbon*, followed by "o", is used as prefix and numbering of the hydrocarbon is continued along the bridge, *cf.* (XVI).



(XIII)
Bicyclo[3,2,1]octane



(XIV)
Bicyclo[3,3,0]oct-2-ene



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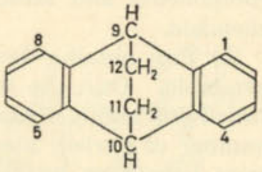


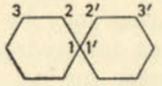
(XV)
9,10-Ethylene-9,10-dihydroanthracene

(XVI)
9,10-Dihydro-9,10-ethanoanthracene

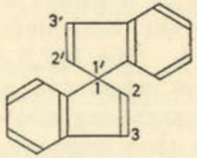
(4) Spirans, if completely symmetrical (excluding substituents), are simply named as, for example, spirobi(cyclohexane) (XVII), or 1,1′-spirobi-indene (XVIII), with primed and unprimed numbers. Unsymmetrical spirans may receive names of the type fluorene-9-spiro-1′-cyclopentane-3′-spirocyclohexane (XIX) (beginning with the most complex constituent). *Chemical Abstracts* uses considerably different methods.

Both sets of methods are accepted, as alternatives, in the I.U.P.A.C. rules.

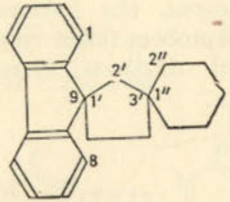
(5) A cyclic hydrocarbon with short side chains is normally treated as a substituted cyclic compound,



(XVII)



(XVIII)

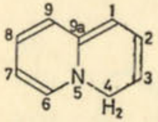


(XIX)

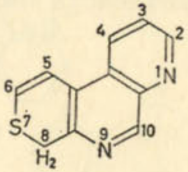
e.g., hexamethylbenzene. A simple ring system with a long side chain is normally treated as a substituted aliphatic hydrocarbon, *e.g.*, 1-phenyldecane. Complex ring systems are normally treated as parents, even if they have long side chains, *e.g.*, 1-dodecylpyrene. Choice is free for intermediate cases (*Chemical Abstracts* considers pentyl short and hexyl long for benzene derivatives). Unsaturation in the side chain tends to favour the side chain as parent, *e.g.*, 1-2′-naphthylhexa-1,3-diene. Chains substituted by two or more cyclic radicals are also most conveniently treated as parents, since, for example, 2-3′-naphthyl-4-phenylhexane is simpler than 2-(1-methyl-3-phenylpentyl)naphthalene. It must, however, always be remembered that presence of a functional group may override any such considerations (see pp. 42, 46).

HETEROCYCLIC COMPOUNDS

There is a great profusion of trivial names for heterocyclic compounds, even when the alkaloids are excluded. The I.U.P.A.C. 1957 rules list names of forty-five heterocyclic skeletons that may be used in fusion operations and of fourteen for hydrogenated systems that may not. All names for heterocyclic compounds can be treated as parent names for use by the spiran or bi-procedure, as for hydrocarbons. In heterocyclic skeletons, the heteroatoms have the lowest available numbers (after rule (*iv*) above), and by the *Chemical Abstracts* system, adopted by I.U.P.A.C., are numbered even if they occur at a fusion (valley) position, as in (XX).



(XX)

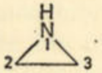


(XXI)

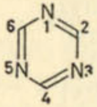
In addition, names may be formed from any hydrocarbon by indicating replacement of a ring member by, for instance, oxygen, sulphur, or nitrogen by oxa-, thia-, aza-prefixes, respectively. The numbering of the hydrocarbon is retained by this procedure, and if more than one kind of heteroatom is present they are cited in a prescribed order (*e.g.*, that just given). An example would be 8*H*-7-thia-1,9-diazaphenanthrene (XXI). This nomenclature must be applied to the hydrocarbon "parent", not to a less

heterosubstituted system—to avoid plurality of names such as, for instance, 4*H*-3-thia-7-azaphenanthridine for (XXI). (In certain cases *Chemical Abstracts* and Beilstein's *Handbuch* use this device in different ways; both are set out, as alternatives, in the I.U.P.A.C. 1957 rules, and both have been used in British work.)

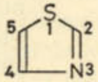
Finally there is the Hantzsch–Widman nomenclature[4] for 5- and 6-membered rings, extended in the *Ring Index* and adopted in the I.U.P.A.C. 1957 rules, by which any monocyclic heterocompound with 3–10 members in the ring can be named in a systematic way. Syllables oxa, thia, aza (as above), *etc.*, denote the heteroatoms and are combined with syllables representing ring size, the positions of the heteroatoms being denoted by numerals. The full rules (see I.U.P.A.C. report) are fairly complex but form a powerful tool; the range is wide, for the names can be used for fusion and with the spiran or bi-procedure; and the final result is always a neat, compact name. Some examples are aziridine (XXII; ir from tri),



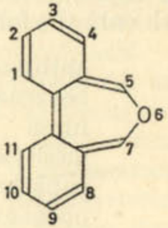
(XXII)



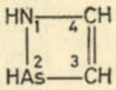
(XXIII)



(XXIV)



(XXV)



(XXVI)

1,3,5-triazine (XXIII), 1,3-thiazole (XXIV), dibenz[*c*,*e*]oxepin (XXV; ep from hepta), and 1,2-arsazetin (XXVI; et from tetra).

RADICALS

Univalent radicals derived from unsaturated alkanes and cycloalkanes are named by changing the ending -ane to -yl. From all other skeletal names, whether of saturated or unsaturated compounds, radical names are formed by merely *adding* -yl to the full name, without elision except of terminal "e", with only the following exceptions:

anthracene	anthryl
benzene	phenyl
furan	furyl
mesitylene	mesityl
naphthalene	naphthyl
phenanthrene	phenanthryl
piperidine	piperidyl
pyridine	pyridyl
quinoline	quinolyl
isoquinoline	isoquinolyl
thiophen	thienyl
toluene	tolyl
	benzyl
xylene	xylyl

REFERENCES

[1] *I.U.P.A.C. Nomenclature of Organic Chemistry*, 1957, Butterworths, London, 1958.

[2] STELZNER, R., *Literatur-Register der organischen Chemie*, Springer, Berlin, 1931, Vol. III, 1914–15, pp. 22–24.

[3] VON BAYER, A., *Ber. dtsch. chem. Ges.*, 1900, **33**, 3771.

[4] HANTZSCH, A. and WEBER, J. H., *Ber. dtsch. chem. Ges.*, 1887, **20**, 3119; WIDMAN, O., *J. prakt. Chem.*, 1888, [2], **38**, 185.

8

ORGANIC: SOME SPECIAL CASES

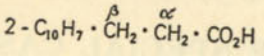
Conjunctive nomenclature

According to this type of nomenclature a name such as 2-naphthalenepropionic acid denotes a naphthalene nucleus linked at position 2 to the *terminal* position of propionic acid with loss of two hydrogen atoms, *i.e.*, the compound (I), which by substitutive nomenclature is called β-naphthylpropionic acid. Its wide use (*cf.* p. 40) by *Chemical Abstracts* for arylaliphatic (aralkyl) compounds with a functional group in the aliphatic portion has led to its fairly common use in American journals and books in circumstances where European authors prefer the older systematic nomenclature. There seems no reason to urge change of the European attitude.

Two features of this nomenclature must be noted. (*i*) The cyclic component receives its usual numbers; the acyclic portion receives Greek letters running from the functional group to the cyclic portion for each carbon atom which can bear a substituent, as in (I) and (II). (*ii*) The main chain is considered to run from the functional group to the cyclic nucleus and is not necessarily the longest chain of the aliphatic component *per se*; *e.g.*, (III) α-ethyl-2-naphthalenepropionic acid.

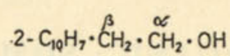
This nomenclature appears justifiable even for Europe in some fairly rare cases where substitutive nomenclature is clumsy or obscures the functional groups. Thus for acid (IV) the name 1,2,3-cyclohexanetriacetic acid may be preferable to 1,2,3-tri-

2′-carboxyethylcyclohexane when the presence of the carboxyl groups is important. It can be usefully



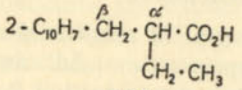
$2\text{-}C_{10}H_7\cdot\overset{\beta}{C}H_2\cdot\overset{\alpha}{C}H_2\cdot CO_2H$

(I)



$2\text{-}C_{10}H_7\cdot\overset{\beta}{C}H_2\cdot\overset{\alpha}{C}H_2\cdot OH$

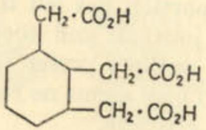
(II)



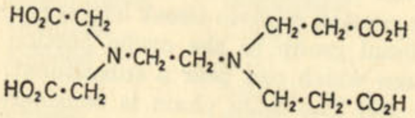
$2\text{-}C_{10}H_7\cdot\overset{\beta}{C}H_2\cdot\overset{\alpha}{C}H(CH_2\cdot CH_3)\cdot CO_2H$

(III)

modified for names of this EDTA type; the "conjunctive name" for (V), ethylenediamine-*NN*-diacetic-*N′N′*-dipropionic acid is easy to understand.



(IV)



(V)

Aliphatic acids

These are numbered with $CO_2H = 1$ when named as -oic acids or by trivial names, though with trivial names of the *lower* members the Greek letters α (=2), β (=3), *etc.*, are used in Great Britain. The three trivial names of acids beginning with capr- should be superseded by the systematic names (caproic = hexanoic, caprylic = octanoic, capric = decanoic). For acids named by the carboxylic acid method, *e.g.*, heptane-3-carboxylic acid or 3-carboxypropylammonium chloride, the CO_2H group is treated by the normal methods for suffixes and prefixes (see p. 46).

Aliphatic alcohols

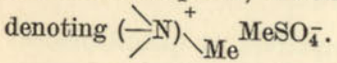
Formation of alcohol names must be carried out systematically. Propan-2-ol is correct; isopropanol is incorrect because there is no parent isopropane from which this name can be derived; isopropyl alcohol is a correct alternative, because there is a radical isopropyl $CHMe_2$— (sodium isopropoxide is similarly correct). Moreover, though there is isobutane, isobutanol is ambiguous whereas isobutyl alcohol is specific (from the radical $CHMe_2\cdot CH_2$—).

Amine salts

Amine salts, being derivatives of quadricovalent nitrogen, should systematically be named as -onium or -inium salts (*cf. Table* 4, p. 48), *e.g.*, $NH_2Et_2^+Cl^-$ diethylammonium chloride, $Ph\cdot NH_3^+Cl^-$ anilinium chloride, $C_5H_6N^+C_6H_2O_7N_3^-$ pyridinium picrate. Much use is, however, still made of names such as aniline hydrochloride, pyridine picrate (note that "hydro" is included only with the halide names: aniline hydrochloride, hydrobromide, or hydriodide, but aniline picrate or nitrate; this old, irrational practice is probably derived from the names for the acids). Such "irregular" names for amine salts are, however, necessary for unsymmetrical bases when the point of attachment of the proton cannot be defined, as in naphthalene-1,6-diamine monohydrochloride (if the point of attachment were known, the specific name would be, *e.g.*, 6-amino-1-naphthylammonium chloride).

Care must be taken with amine salts of dibasic acids: *e.g.*, $Ph\cdot NH_3^+HSO_4^-$ is anilinium hydrogen sulphate, $(Ph\cdot NH_3^+)_2SO_4^{2-}$ is dianilinium sulphate, whereas aniline sulphate or anilinium sulphate might refer to either salt.

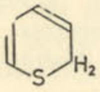
Quaternary salts have systematic names such as triethylmethylammonium chloride, *NNN*-trimethylanilinium bromide, 1-methylquinolinium picrate. Quaternary salts are, however, often handled by an older method, as metho-salts, *e.g.*, triethylamine methochloride, quinoline methopicrate: this older method should not normally be used, though it is useful for compounds of uncertain composition (*cf.* hydrochloride, *etc.*). Salts derived by addition of Me_2SO_4 are named after the pattern of 1-methylpyridinium methyl sulphate or naphthalene-1,6-diamine monomethosulphate, the trivial name methosulphate denoting



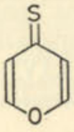
$$(\gtrdot\overset{+}{N})\diagdown_{Me}\ MeSO_4^-.$$

Thio-compounds

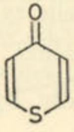
The nomenclature of compounds containing —S— and =S is unsatisfactory. As stated in the list on p. 48, —SH is denoted by the suffix -thiol (which is also the generic name) or prefix mercapto-, whereas MeS— is methylthio-; sulphides, *e.g.*, MeSBu, are named as methylthiobutane or butyl methyl sulphide. "Thioketones" RR′C=S may be named by the suffix -thione (used in the same way as -one, as in $MeBu^nC{=}S$ hexane-2-thione); the prefix may be thiono-, though thioxo- is usual in America. In addition, a prefix thio- is widely used to denote replacement of oxygen by sulphur, particularly for acids and phenols (*cf.* thioketones and thioxo-; also inorganic practice, p. 19). Thiophenol and thiocresol are normally used for PhSH and $C_6H_4Me\cdot SH$, respectively (although the more systematic names would be benzenethiol and, *e.g.*, toluene-*o*-thiol), and thiophenoxide or thiophenoxy- for the radical PhS—. Thiobenzoic acid and dithiobenzoic acid for Ph·COSH and $Ph\cdot CS_2H$ illustrate widespread usage. The I.U.P.A.C. 1932 rules[1] recommend names such as ethanethiolic Me·C(:O)·SH, ethanethionic Me·C(:S)·OH, ethanethionothiolic $Me\cdot CS_2H$ (here ethanedithioic would surely be adequate), and ethanethioic for indeterminate Me·CSOH (which is the case for all the acids but not, of course, for the esters); carbothiolic, carbothionic, and carbothionothiolic are the carboxylic equivalents; however, the 1961 tentative rules suggest alternative procedures.



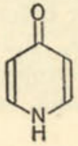
(VII)



(VIII)



(IX)



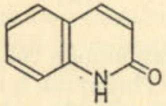
(X)

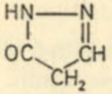
Particular care is needed with compounds containing two kinds of oxygen atom. 2*H*-Thiopyran is often used for compound (VII) (the *Ring Index* prefers thiapyran, though this is, strictly, misuse of thia as at present defined). It is easy to confuse the sulphur analogues, such as (VIII) and (IX), of 4-pyrone: it seems best here to abandon contractions and use pyran-4-thione (VIII) and thiopyran-4-one (or thiacyclohexan-4-one) (IX). There are several similar cyclic cases, *e.g.*, thiochromen, thioxanthen. And there is one particular offender in the aliphatic series: $HS\cdot CH_2\cdot CO_2H$ is widely named thioglycollic acid, derived from glycollic acid $HO\cdot CH_2\cdot CO_2H$; this thio-name, which could equally apply to

$HO\cdot CH_2\cdot CSOH$, should be abandoned; mercaptoacetic acid is unambiguous and correct.

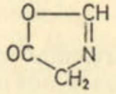
Heterocyclic ketones

Certain long-established names such as 4-pyridone (X) and 2-quinolone (XI) not merely have abbreviated endings but actually refer to ketones derived from dihydro-derivatives. Other long-established names such as pyrazolone (XII) and oxazolone (XIII), though not abbreviated, also refer to ketones from dihydro-derivatives. This would give the names 1,4-dihydropyridin-4-one, 1,2-dihydroquinolin-4-one, 4,5-dihydropyrazol-5-one, *etc.* This irregularity has been rather widely extended, in two directions: first to other heterocyclic systems generally, so that, for example, 1,2-dihydro-2-oxopyrazine (alternatively, 1,2-dihydropyrazin-2-one) (XIV) becomes pyrazin-6-one, and secondly by *Chemical Abstracts* to diketones, triketones, *etc.*, so that 1,2,3,4-tetrahydro-2,4-dioxopyridine (XV) becomes 1,3*H*-pyridine-2,4-dione, and 2,3-dihydro-2,3-dioxopyridine (XVI) becomes pyridine-2,3-dione (note the disparity in reduction stages, indicated only by the *H*-prefixes). Use of hydro- and oxo- prefixes is recommended for British work, except for very long-established names.

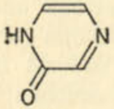

(XI)



(XII)



(XIII)



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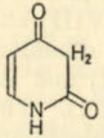

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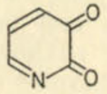


(XVI)

Carbonyl derivatives

Compounds $>C{=}X$ derived from ketones or aldehydes $\left(>C{=}O\right)$ are named as two words, thus acetone semicarbazone, acetophenone 2,4-dinitrophenylhydrazone, benzoin monoxime or dioxime, *p*-benzoquinone di-imine. Names of simple oximes are often abbreviated, *e.g.*, to acetoxime (acetone oxime) or benzaldoxime, but the few common examples should be regarded as trivial names and not as patterns for a general abbreviation.

Trityl- $(-CPh_3)$

This may be used as a prefix in names of steroid and carbohydrate derivatives, but *not* in forms such as trityl chloride or trityl alcohol.

Tosyl- (toluene-*p*-sulphonyl)

Tosyl is permitted as a prefix in organic names, but *not* in forms such as toxyl chloride or tosylate. Pipsyl and analogous short cuts are not approved, though mesyl is sanctioned in the I.U.P.A.C. 1961 tentative rules.

Metallo-organic compounds

The same names are used in organic as in inorganic chemistry: *e.g.*, phenylsodium, ethyl-lithium, dimethylmercury (*not* sodium phenyl, lithium ethyl, or mercury dimethyl); methylmercuric bromide; chloromercuribenzoic acid ($ClHg{\cdot}C_6H_4{\cdot}CO_2H$).

Stereochemistry

Use of *cis-*, *trans-*, *syn-*, *anti-*, *amphi-*, *cisoid*, and *transoid* is adequately covered in standard textbooks.

D-, L-, and DL- (roman small capital letters) *must* be reserved solely for compounds containing only one asymmetric carbon atom which can be unambiguously correlated with glyceraldehyde (this has known absolute configuration), and for proteins and carbohydrates (and closely related compounds) where D- and L- are used in specialized manners, covered by adequate reports[2]. For all other compounds (+)-, (−)-, and (±)- should be used. Fischer's use of *d*- and the carbohydrate chemists' use of L- for dextrorotatory tartaric acid leads to repeated confusion: it is thus preferable to use (+)- and (−)- for the active tartaric acids. The meaning and use of racemic and *meso-* are simple.

For the specification of absolute configuration in other cases the present author naturally favours the sequence rule[3].

When a ring can be reasonably drawn in the plane of the paper, a heavy continuous line attached to the ring represents a bond projecting in front of the plane of the paper, and a broken or dotted line a bond projecting behind this plane. For such cyclic compounds which have a well-established orientation, bonds projecting behind the plane are denoted α and those projecting to the front are denoted β. For steroids and terpenes these designations represent also the absolute configurations. An occasional bond of unknown configuration is represented by a wavy line and designated ξ (xi).

The terms axial (*ax*) and equatorial (*eq*) are now standard for use with conformations.

MISCELLANEOUS

The following reports and rules should be consulted by chemists working in the respective fields. They are reproduced in the "Handbook for Chemical Society Authors", Special Publication No. 14, issued by The Chemical Society, Burlington House, London, W.1.

Monoterpene hydrocarbons: covered by a section of the I.U.P.A.C. rules[4].

Steroids: covered by definitive rules issued jointly by the Commissions on the Nomenclature of Organic and Biological Chemistry with the I.U.P.A.C. 1957 rules[4]. They revise the earlier "tentative" version and differ chiefly in reducing the principal nomenclature to four parents to be used always with 5α- or 5β-. They cover also specialized uses of nor and seco which are useful also in other fields.

Carbohydrates: covered by a British-American agreement[2(b)].

Organophosphorus compounds: a dangerous divergence of British and American practice was rectified by a compromise agreement embodying some new conceptions[5].

Polyhalogeno-compounds: covered by American rules which have been adopted also in Great Britain[6].

Vitamins: some are covered by definitive I.U.P.A.C. rules[7], and the vitamin B_{12} field by tentative rules published by the Commission on the Nomenclature of Organic Chemistry with the 1957 rules[4].

Labelled compounds: symbolism has been agreed between The Chemical Society and the Biochemical Society[8].

General biochemistry: in biochemical matters (in cluding symbols for amino-acids) the Biochemical Society's *Suggestions to Authors* (revised in 1962) should be followed.

REFERENCES

[1] *Cf. J. chem. Soc.*, 1952, 5068 (rule 30).

[2](a) Amino-acids: *I.U.P.A.C. Comptes rendus of the 15th Conference*, 1949 pp. 187–189; *J. chem. Soc.*, 1951, 3522–3524

(b) Carbohydrates: *J. chem. Soc.*, 1952, 5108–5121.

[3] Cahn, R. S., Ingold, C. K., and Prelog, V., *Experientia*, 1956, **12**, 81–94.

[4] *I.U.P.A.C. Nomenclature of Organic Chemistry*, 1957, Butterworths, London, 1958.

[5] *J. chem. Soc.*, 1952, 5122–5131.

[6] *J. chem. Soc.*, 1952, 5059–5060.

[7] *I.U.P.A.C. Comptes rendus of the 14th Conference*, 1951, pp. 142–143; *17th Conference*, 1953, pp. 149–150: *cf. J. chem. Soc.*, 1951, 3525–3526; 1954, 4719.

[8] *Quart. Rev. chem. Soc., Lond.*, 1957, **7**, 407; *J. chem. Soc.*, 1953, 4203–4204.

9

PHYSICOCHEMICAL SYMBOLS

(*Names of independent quantities are separated by colons; alternative names for a single quantity are separated by semicolons. Enclosure of the name of a quantity in parentheses indicates that there is an alternative symbol of equal standing; enclosure in square brackets indicates that there is another symbol which is preferred. An asterisk against the name of a quantity indicates that the specified symbol is always used with a subscript when denoting that quantity.*)

A	area: atomic weight
$\mathbf{A}$, A	magnetic vector potential
a	acceleration: activity, relative
B	(luminance; brightness): susceptance
$\mathbf{B}$, B	magnetic flux density; magnetic induction
b	breadth
C	heat capacity per mole: (concentration): capacitance
c	heat capacity per unit mass: (concentration)
$\boldsymbol{c}$, c	speed of light
D	differential operator
D	diffusion coefficient
$\mathbf{D}$, D	electric flux density; electric displacement
d	differentiation
∂	partial differentiation
d	diameter: relative density: current density at an electrode surface
E	(energy): Young's modulus: activation energy: illumination: electromotive force: single electrode potential*
$\mathbf{E}$, E	electric force; electric field strength
e	base of natural logarithms
$-\boldsymbol{e}$, $-e$	charge of electron
F	force: free energy; Helmholtz function: (luminous flux)
$\boldsymbol{F}$, F	Faraday's constant
f	(frequency): [acceleration]: (activity coefficient)

G	rigidity: Gibbs function: conductance
$\boldsymbol{G}$, G	gravitational constant
g	gravitational acceleration: osmotic coefficient
$\mathbf{g}$, g_0	gravitational acceleration, standard value
H	heat function; enthalpy; total heat
$\mathbf{H}$, H	magnetic field strength; magnetizing force
h	height
$\boldsymbol{h}$, h	Planck's constant
$\mathbf{I}$, I	[intensity of magnetization]
I	moment of inertia: luminous intensity: electric current: ionic strength
i	(square root of minus one)
$\mathbf{J}$, J	current density
j	(square root of minus one)
K	bulk modulus: equilibrium constant of chemical reaction
k	radius of gyration: (thermal conductivity): velocity constant of chemical reaction
$\boldsymbol{k}$, k	Boltzmann's constant
L	(luminance; brightness): inductance, especially self-inductance: inductance, self or mutual*
	length: [equivalent ionic conductance*]
$\mathbf{M}$, M	(intensity of magnetization)
M	moment: bending moment: molecular weight: mutual inductance
M	molarity: molar
m	mass: molality: molal
$\boldsymbol{m}$, m	mass of electron
$\boldsymbol{N}$, N	Avogadro's number
N	number of molecules
N	normality: normal
n	number of moles: refractive index*
P	(pressure): power
p	(pressure)
Q	(quantity of heat): electric charge: power, reactive: partition function
q	(quantity of heat)
$\boldsymbol{R}$, R	gas constant per mole: Rydberg's constant
R	luminous radiance: resistance
r	radius: spherical or cylindrical co-ordinate: (resistivity; specific resistance)

S	entropy: power, apparent
$\mathbf{S}$, S	Poynting vector
T	period: kinetic energy: torque: temperature, absolute: (transport number*)
t	time: [temperature, empirical]: (transport number*)
U	internal energy
u	(velocity)
V	(volume): potential energy: potential: potential difference: (electromotive force)
v	(volume): (velocity)
W	weight: (work): (energy): energy, electrical
w	(work): weight fraction
X	reactance
x	co-ordinate: mole fraction
Y	admittance
y	co-ordinate
Z	modulus of section: atomic number: impedance
z	co-ordinate: valency of an ion
α	(angle): angular acceleration: coefficient of thermal expansion: degree of dissociation: light absorption factor
β	(angle): luminance factor
$\boldsymbol{\beta}$, β	Bohr's magneton
Γ	surface concentration
γ	(surface tension): ratio of specific heats: (activity coefficient, especially stoicheiometric): conductivity; specific conductance)
Δ	increment or finite difference operator
δ	increment or finite difference operator: dielectric loss angle
ε	[base of natural logarithms]: permittivity
ζ	electrokinetic potential
η	efficiency: viscosity: electrolytic polarization; overpotential
θ	(angle): spherical co-ordinate: temperature, empirical
$\varkappa$	compressibility: magnetic susceptibility, volume: conductivity; specific conductance, especially of electrolytes
Λ	equivalent conductance: equivalent ionic conductance*

λ	wave-length: (thermal conductivity): activity, absolute
μ	coefficient of friction: Joule–Thomson coefficient: chemical potential: [refractive index *]: permeability: dipole moment
ν	(frequency): (wave number): [Poisson's ratio]: kinematic viscosity: stoicheiometric number of molecules
$\tilde{\nu}$	(wave number)
Π	product
$\mathit{\Pi}$	osmotic pressure
π	ratio of circumference to diameter
ρ	density: light reflexion factor: electric charge density, volume: (resistivity; specific resistance)
Σ	summation
σ	Poisson's ratio: (surface tension): electric charge density, surface: (conductivity; specific conductance)
$\boldsymbol{\sigma}$, σ	Stefan–Boltzmann constant
τ	light transmission factor
Φ	(luminous flux): magnetic flux
ϕ	(angle): spherical or cylindrical co-ordinate: fluidity: electronic exit work function: phase difference: volume fraction
χ	magnetic susceptibility, mass
Ψ	electric flux
ψ	(angle)
ω	solid angle: angular velocity

General

The above list gives the symbols recommended by the Symbols Committee of the Royal Society (1951). This embodies the usage, which should be employed for all symbols, that italic letters denote physical quantities (area, equilibrium constants, density, *etc.*), bold italic type denotes fundamental constants (gravitational constant, Planck's constant, *etc.*), roman type denotes mathematical operators (d, log, *etc.*), and bold roman type (or ordinary italic) denotes vectors. Units of measurement (cm., ml., *etc.*) should be in ordinary roman type.

Spectral notation

This has been covered by report from a Joint Commission for Spectroscopy of the International Astronomical Union and the International Union of Pure and Applied Physics[1].

REFERENCE

[1] *J. chem. Phys.*, 1955, **11**, 1997–2011.

10

EXERCISES

Some of the exercises below merely illustrate the principles set out in the preceding chapters. Others, however, concern ways in which these principles may be applied in situations not specifically covered in the earlier text. This being so, it is perhaps wise to emphasize again that the present book is only an introduction to a subject that often becomes very complex—namely provision of specific, different names for each of 2–3 million chemical compounds—and that further study of the texts cited and of the names used by previous workers is essential before more complicated nomenclature is attempted.

Chapter 2

QUESTION 1. What is denoted by the formula $D^{15}N^{14}N_2$?

QUESTION 2. What is denoted by the symbol $[^{18}OH]^-$?

QUESTION 3. If a decimal point is used to denote a free electron, what is the symbol for a hydrogen molecule ion?

ANSWER 1. A hydrogen azide (hydrazoic acid) molecule containing one atom of deuterium, one atom of nitrogen-15, and two atoms of nitrogen-14 (p. 7).

ANSWER 2. A hydroxyl ion containing the isotope oxygen-18 (p. 7). Note: strictly, no oxygen-16 should be present, but this symbolism is also commonly used for labelled ("tagged") species, so that $[^{18}OH]^-$ is often used for the ion containing only a slightly reinforced proportion of the rare isotope oxygen-18. Such situations are normally immediately evident from the text, but much care may be needed in interpreting formulae such as that given in the questions.

ANSWER 3. $H_2\cdot$ (p. 7).

QUESTION 4. Why is it correct to write dichlorine oxide but oxygen difluoride?

QUESTION 5. Name the compound $SnCl_4$.

QUESTION 6. Derive the formula for tetroxorhenic(V) acid.

QUESTION 7. Why is it correct to write zirconium oxide dichloride for $ZrOCl_2$ but vanadyl(IV) chloride for $VOCl_2$?

ANSWER 4. Because, for compounds between two elements, the I.U.P.A.C. rules specify prior citation of atoms placed first in a specified list which includes the order I, Br, Cl, O, F (p. 9).

ANSWER 5. The old-fashioned name is stannic chloride, and this is still widely used. According to the I.U.P.A.C. rules it would be termed tin tetrachloride or tin(IV) chloride; actually the rules indicate a preference for stannum(IV) chloride (p. 2), but Latin names are in fact rarely used for the common metals and are not favoured by the Chemical Society (p. 12). Note, however, that the Latin roots are used for ions containing these metals as one element therein, *e.g.*, stannate.

ANSWER 6. In tetroxorhenic(V) acid, there are four atoms of (bivalent) oxygen; the rhenium atom is quinquevalent (denoted by V), so there remain three of the total of eight oxygen valencies to be satisfied by hydrogen. The formula is therefore H_3ReO_4 (p. 21).

ANSWER 7. The only oxygen-containing radical names that are sanctioned for inorganic compounds are those listed on p. 23. Vanadyl is in this list, but not zirconyl, so that $ZrOCl_2$ is treated as an oxide salt. The (IV) in the vanadyl name is added because vanadyl(V) and vanadyl(VI) compounds are known. The "di" in zirconium oxide dichloride is optional and may be omitted if the quadrivalency of zirconium is assumed.

Chapter 3

QUESTION 8. Alphabeticize the prefixes in the following names:

(*a*) 4-Diethylamino-2-ethyl-6-ethylaminophenol
(*b*) 2,7-Dimethyl-3-fluoro-4-bromooctane
(*c*) 6-Methyl-4-dimethylamino-3,6,10,12,12a-pentahydroxy-1,11-dioxo-1,4,4a,5,5a,6,11,12a-octahydronaphthacene-2-carboxyamide.

ANSWER 8. (*a*) As given.
(*b*) 4-Bromo-3-fluoro-2,7-dimethyloctane.
(*c*) 4-Dimethylamino-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxonaphthacene-2-carboxyamide.

According to the I.U.P.A.C. 1961 tentative rules,

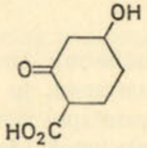
"hydro" may be alphabeticized or kept next to the name of the parent compound; in England and U.S.A. it should always be alphabeticized.

Chapter 4

QUESTION 9. State the principal functional group (for citation as suffix) in the following compounds, and hence derive the names.

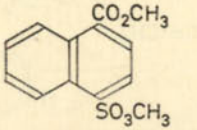
(*a*) $CH_3{\cdot}CO{\cdot}CH_2{\cdot}CH_2{\cdot}CH(OH){\cdot}CH_3$

(*b*)



(*c*)

(*d*)



(*e*) $CH_3O{\cdot}CH_2{\cdot}CH_2{\cdot}CH_2{\cdot}SH$

ANSWER 9. The answers are all based on *Table 4* (pp. 48–49).

(*a*) 5-Hydroxyhexan-2-one
(*b*) 4-Hydroxy-2-oxocyclohexanecarboxylic acid
(*c*) *p*-Aminophenol
(*d*) Methyl 4-methoxysulphonylnaphthoate
(*e*) 3-Methoxypropane-1-thiol.

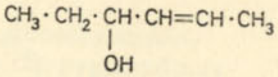
It will be seen that the oxygen group is chosen for suffix in example (*d*), but the sulphur group in example (*e*). This is because esters rank for priority immediately after their respective acids, so that for (*d*) carboxylate and not sulphonate is the principal functional group, and this is not altered because the systematic naphthalenecarboxylate is abbreviated to naphthoate; however, ether and sulphide groups both rank after alcohols, phenols, and thiols—the rule in fact has considerable empiricism in its make-up.

Chapter 5

QUESTION 10. Remembering that (see pp. 53–54) lowest numbers are assigned, in sequence as far as necessary, to (*a*) the principal functional group, (*b*) a double bond, (*c*) a triple bond, (*d*) prefixes considered together as a series of numbers, and (*e*) prefixes cited first in alphabetical order, number the following compounds:

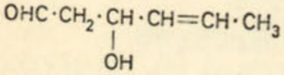
$CH_3\cdot CH_2\cdot CH_2\cdot CH{=}CH\cdot CH_3$

(I)



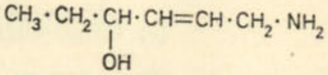
$CH_3\cdot CH_2\cdot \underset{OH}{CH}\cdot CH{=}CH\cdot CH_3$

(II)



$OHC\cdot CH_2\cdot \underset{OH}{CH}\cdot CH{=}CH\cdot CH_3$

(III)



$CH_3\cdot CH_2\cdot \underset{OH}{CH}\cdot CH{=}CH\cdot CH_2\cdot NH_2$

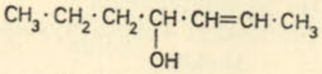
(IV)

$Br\cdot [CH_2]_8\cdot Cl$

(V)

$Br\cdot CH_2\cdot CH_2\cdot CH{=}CH\cdot CH_3$

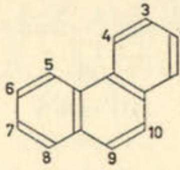
(VI)



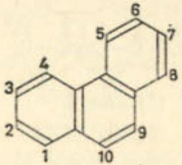
$CH_3\cdot CH_2\cdot CH_2\cdot \underset{OH}{CH}\cdot CH{=}CH\cdot CH_3$

(VII)

QUESTION 11. The numberings (A) and (B) are equivalent for phenanthrene:

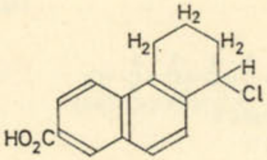


(A)

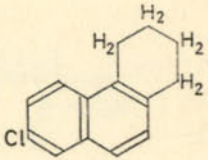


(B)

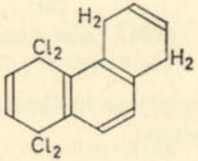
Number the following compounds:



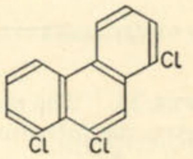
(VIII)



(IX)

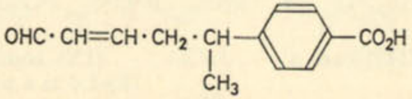


(X)

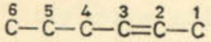


(XI)

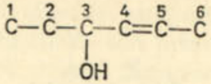
QUESTION 12. Number the side chain in the following compound:



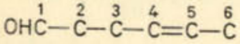
Answer 10. Only the atoms necessary to decide the numbering are given below.


$\overset{6}{C}-\overset{5}{C}-\overset{4}{C}-\overset{3}{C}=\overset{2}{C}-\overset{1}{C}$

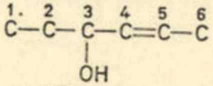
(I) case *b*


$\overset{1}{C}-\overset{2}{C}-\underset{\mathrm{OH}}{\overset{3}{C}}-\overset{4}{C}=\overset{5}{C}-\overset{6}{C}$

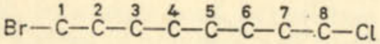
(II) case *a*


$\mathrm{OH}\overset{1}{C}-\overset{2}{C}-\overset{3}{C}-\overset{4}{C}=\overset{5}{C}-\overset{6}{C}$

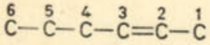
(III) case *a*


$\overset{1.}{C}-\overset{2}{C}-\underset{\mathrm{OH}}{\overset{3}{C}}-\overset{4}{C}=\overset{5}{C}-\overset{6}{C}$

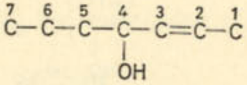
(IV) case *a*


$Br-\overset{1}{C}-\overset{2}{C}-\overset{3}{C}-\overset{4}{C}-\overset{5}{C}-\overset{6}{C}-\overset{7}{C}-\overset{8}{C}-Cl$

(V) case *e*

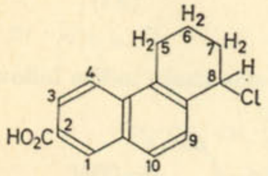

$\overset{6}{C}-\overset{5}{C}-\overset{4}{C}-\overset{3}{C}=\overset{2}{C}-\overset{1}{C}$

(VI) case *b*

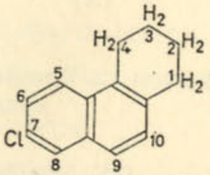

$\overset{7}{C}-\overset{6}{C}-\overset{5}{C}-\underset{\mathrm{OH}}{\overset{4}{C}}-\overset{3}{C}=\overset{2}{C}-\overset{1}{C}$

(VII) cases *a* and *b*

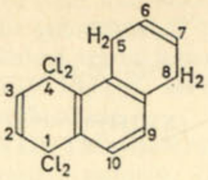
Answer 11. The same rules apply as in Question 10 and give the following numberings:



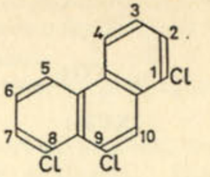
(VIII) case *a*



(IX) case *d*
(hydro is a prefix)

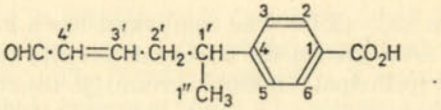


(X) case *e*



(XI) case *d*
(1,8,9 is lower than 1,8,10)

Answer 12. The point of attachment of a radical (side chain) always has number 1, so that the numbering is:



Chapter 6

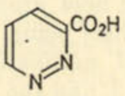
Question 13. Describe the approach to names of the following compounds:

$CH_3\cdot CO\cdot CH_2\cdot CH_2\cdot O\cdot CO\cdot C_6H_5$

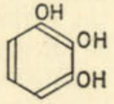
(XII)

$CH(CH_2\cdot CH_2\cdot OH)_3$

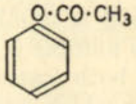
(XIII)



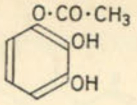
(XIV)



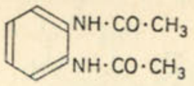
(XV)



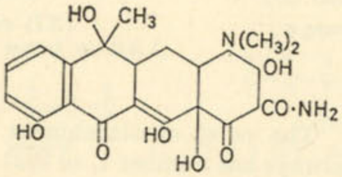
(XVI)



(XVII)



(XVIII)



(XIX)

ANSWER 13. (XII) The compound has a ketone and and an ester group; the latter has priority for citation as suffix (principal functional group) (p. 48), so the compound is named as an ester of benzoic acid and the keto-alcohol $CH_3{\cdot}CO{\cdot}CH_2{\cdot}CH_2{\cdot}OH$. In naming the radical $CH_3{\cdot}CO{\cdot}CH_2{\cdot}CH_2–$ the point of attachment carries number 1. So the name is 3-oxobutyl benzoate.

(XIII) This is example (VIII) on p. 58, written in another form.

(XIV) The heterocyclic base is pyrazine, whose two nitrogen atoms must be numbered 1 and 2. However, the carboxylic acid group has priority over amine groups for citation as suffix, so the name must end in carboxylic acid, and this group must not be cited by the prefix carboxy. According to which way round the ring is numbered, the carboxylic acid group receives number 3 or 6 (the nitrogen atoms being 1 and 2 in both cases). The direction of numbering is chosen which gives the lower number 3, and the name is thus pyrazine-3-carboxylic acid.

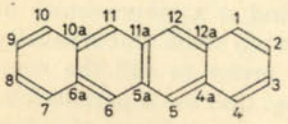
(XV) The systematic name is benzene-1,2,3-triol, but the compound is usually known by its very well-established trivial name pyrogallol.

(XVI) Phenyl acetate is clearly preferable to acetoxybenzene.

(XVII) This illustrates the sort of problem met so frequently, namely, conflicting analogies. Analogy with the preceding example, phenyl acetate (XVI), indicates the systematic name 2,3-dihydroxyphenyl acetate for (XVII) and it would not be wrong to use this name. Yet the compound is a monoacetate of pyrogallol; and since the latter is a name that is usually used, many chemists would prefer to call the compound pyrogallol 1-acetate, and that too is permissible. However, by analogy with the nomenclature of polyol esters used in carbohydrate chemistry (*cf.* p. 85) and elsewhere, the name 1-*O*-acetylpyrogallol should be permissible. The fourth possibility, 3-acetoxypyrocatechol, has, however, nothing to recommend it.

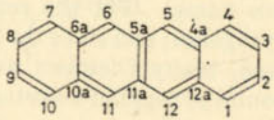
(XVIII) The compound is an amide. If we use the priority table on p. 49, the name might end in -amide; the diradical $C_6H_4<$ is phenylene, so *NN'*-*o*-phenylenebisacetamide or *NN'*-phenylenedi(acetamide) is a possibility. [Note, in passing, the exact form of these two endings, adopted to avoid confusion with diacetamide, which has the structure $NH(CO{\cdot}CH_3)_2$.] The compound (XVIII) is, however, perhaps more easily recognized as the diacetyl derivative of *o*-phenylenediamine, and there is no objection to the name, *NN'*-diacetyl-*o*-phenylenediamine; but note that when an amide is named as an acylamine the ending amine and not amide is used.

(XIX) This is the antibiotic tetracycline and that name can be used. It is, however, not difficult to derive the systematic name if one has one piece of specific knowledge that can easily be obtained from the I.U.P.A.C. rules or from the Ring Index. First one looks for the principal functional group and finds it to be the amide group (*Table* 4), so that the name ends in carboxyamide. This group is attached to a tetracyclic nucleus; the specific piece of knowledge mentioned above is that the aromatic parent of this ring system is called naphthacene, which is numbered as (C) (equivalent to C′). The carboxyamide group must be assigned the lowest available number, so that the numbering as in C′ must be used, which gives this group the number 2 (not 3). The other substituents are then named as prefixes, written with their positional numerals, and arranged in alphabetical order. The result is the name given in the answer to Question 8(*c*) above.



(C)

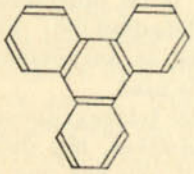
≡



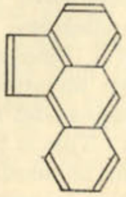
(C′)

Chapter 7

QUESTION 14. Number the following compounds according to the Ring Index system:

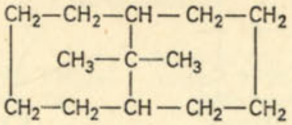


(XX)

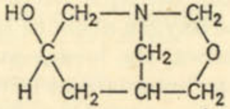


(XXI)

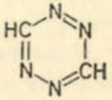
QUESTION 15. Name the compounds



(XXII)

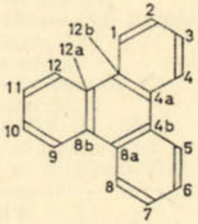


(XXIII)

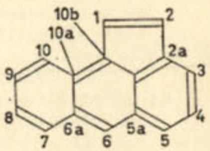


(XXIV)

ANSWER 14. It is necessary first to reorientate formulae (XX) and (XXI) as described on p. 66, and then to number them from the top right-hand ring, with a,b numbers for the ring-junction (valley) positions:

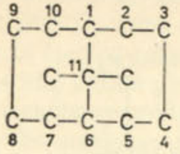


(XX)

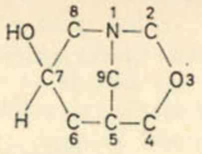


(XXI)

ANSWER 15. Compounds (XXII) and (XXIII) are typical bridged-ring compounds (see pp. 71–72). Numbering of (XXII) offers no difficulty,



(XXII)



(XXIII)

and the name is 11,11-dimethylbicyclo[4,4,1]undecane.

In compound (XXIII) the nitrogen atom in the ring is named as aza and the oxygen atom as oxa (see p. 75). Numbering is as shown, the lowest available numbers being assigned to the heteroatoms in the ring (*i.e.*, N = 1, not 5; O = 3, not 7), notwithstanding that this leads to a high number for the principal functional group. The name is 3-oxa-1-azabicyclo[3,3,1]nonan-7-ol.

Compound (XXIV) is a clear case for the Hantzsch–Widman procedure (p. 75). The ending -ine denotes a nitrogenous six-membered ring, so the name is 1,2,4,5-tetrazine.

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