EDITORIAL REPORT ON NOMENCLATURE, 1956.*

INTRODUCTION

These Reports are designed to collect each year changes in chemical nomenclature, and new nomenclature, adopted by The Chemical Society, provided that these have general interest or application. The present Report is again short and is confined to isolated items. This is not because there are no longer major problems in nomenclature requiring resolution—one has only to consider compounds such as tropolones or sydnones where the classical valency-bond conceptions and the nomenclature based thereon are inadequate, higher terpenes, enzymes, organic compounds requiring by present rules two suffixes (while only one is permitted), metal carbonyls, organoboron compounds, stereoisomerism, etc., or the more complex members of the series not covered by the existing carbohydrate or steroid rules. That no definitive rules have yet been formulated for these and many other cases is not due to the problems' being overlooked, or fully to lack of time for their consideration, or to the difficulties (real though they often are) of obtaining agreement among specialists from different countries. Work continues both at a national and at an international level, but progress is slow.

INORGANIC

Elements.—The Table of International Atomic Weights, 1955, given on p. 4989, includes the internationally recognized names of the elements. The transuranium elements listed are: neptunium (93), plutonium (94), americium (95), curium (96), berkelium (97), californium (98), and mendelevium (101). The names einsteinium and fermium which have been proposed for elements of atomic number 99 and 100 respectively have not yet received I.U.P.A.C. approval.

Complex Boric Acids.—The acid $H[B(HSO_4)_4]$ has been called tetra(hydrogen sulphato)boric acid (*J.*, 1956, 1925). This name, though cumbrous, appears accurate and descriptive, and this type of name should be extensible to analogous compounds and ions.

PHYSICAL

Notation for Spectra of Polyatomic Molecules.—The report on this subject from the Joint Commission for Spectroscopy of the International Astronomical Union and the International Union of Pure and Applied Physics (1954) has been published in *J. Chem. Phys.*, 1955, **23**, 1997. The notation there given should be adopted by authors for The Chemical Society's publications.

Rad.—The International Commission on Radiological Units has recently recommended (*Brit. J. Radiology*, 1954, **27**, 243) that the general unit of absorbed dose, for all types of ionising radiation, should be the rad, of 100 ergs per gram (cf. *Ann. Reports*, 1955, **52**, 44).

Demal.—The use of this description is increasing. A demal solution (D-solution) was originally defined as one containing 1 mole of solute per cubic decimeter of solution, in air at 0° (Parker and Parker, *J. Amer. Chem. Soc.*, 1924, **46**, 312; cf. J., 1956, 4464).

ORGANIC

Organophosphorus Compounds.—The American–British nomenclature for compounds containing one phosphorus atom (*J.*, 1952, 5122) has proved generally adequate in providing unambiguous names for compounds of this class, though the unfamiliarity and complexity of some aspects of these rules have as yet prevented their wide adoption in other countries. One gap has recently been disclosed: the rules do not prescribe for ions of the type PY_6^-. When

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* Reprints of this Report, and of those for each of the years 1950, 1951, 1953—55, may be obtained from the General Secretary, The Chemical Society, price 1*s*. each (post free). It is regretted that the Report for 1952 is out of print.

these were encountered (see *J.*, 1956, 3043) recourse was had to the I.U.P.A.C. Tentative Rules for inorganic nomenclature; for instance, the compound $[(PhO)_4P]^+[(PhO)_3PCl_3]^-$ was named tetraphenoxyphosphonium triphenoxytrichlorophosphate, and others of the series analogously (cf. *J.*, 1956, 3051).

The ways in which some difficulties with compounds containing more than one phosphorus atom have been overcome are sufficiently illustrated by the following examples: *O*-benzylphosphorous *OO*-diphenylphosphoric anhydride for $Ph{\cdot}CH_2{\cdot}O{\cdot}P(OH){-}O{-}PO(OPh)_2$ (*J.*, 1956, 3459); P^1-cytidine-5′ P^2-glycerol-1 pyrophosphate (the systematic name for "cytidine diphosphate glycerol"), where one phosphorus atom in pyrophosphoric acid is combined in an ester group at the 5′-position of cytidine, and the other in an ester group at the 1-position of glycerol (*J.*, 1956, 4186; cf. cytidine diphosphate ribitol, *J.*, 1956, 4583).

$-SF_3$ *and* $-SF_5$ *Groups.*—Classical procedures provide no prefix for naming these groups in organic compounds. The difficulty is that the prefix sulpho refers to $-SO_3H$, and the English sulphuro (as in trifluorosulphuro) is singularly ill adapted for use in other languages (cf. French "soufre," German "Schwefel"). Although thio as a prefix refers strictly to the bivalent group $-S-$ (as in methylthio- for $MeS-$), it was in fact used (*J.*, 1956, 2684) as a basis in the names αα-difluoro-α-(trifluorothio)acetic acid for $SF_3{\cdot}CF_2{\cdot}CO_2H$ and chlorodifluoro(pentafluorothio)methane for $CClF_2{\cdot}SF_5$; for the latter substance the alternative name, chlorodifluoromethylsulphur pentafluoride, was also given [it might have been better to write (chlorodifluoromethyl)sulphur pentafluoride, *i.e.*, with parentheses].

Peptides and Other Oligomers.—Some peculiar problems arise in naming substituted oligomers of precisely known structure. For example, glycylglycylalanine substituted on each nitrogen atom by an acetyl group would be most conveniently named *NN′N″*-triacetylglycylglycylalanine, the acetyl groups being all assembled into one prefix as indeed is good practice if glycylglycylalanine is treated as a single trivial name. Similarly, it appears simple to write *SS′*-dibenzyl-L-cysteinyl-L-cysteine. But, when, as in a recent paper (*J.*, 1956, 3148), substitution becomes more involved, and particularly when it is asymmetric, more readily intelligible names are obtained by treating each monomer unit as a separate complete nomenclature unit, serially, as in *S*-benzyl-*N*-benzyloxycarbonyl-L-cysteinyl-*S*-benzyl-L-cysteine benzyl ester. Occasionally it is even helpful (cf. *J.*, 1956, 3150) to insert additional hyphens, as in *S*-benzyl-*N*-benzyloxycarbonyl-L-cysteinyl-glycylglycine. In default of such devices there may be ambiguity as to which monomer unit is implied by *N*, *N′*, *N″*, *S*, *S′*, etc. Similar problems (and solutions of them) may arise for oligosaccharides or polyesters or polylactones.

Attention may also be drawn to the abbreviations for amino-acids used by The Chemical Society (cf. *J.*, 1956, 3697), following the practice of the Biochemical Society (cf. also Brand and Edsall, *Ann. Rev. Biochem.*, 1947, **16**, 224). These abbreviations are to be used only for construction of abbreviated structural formulæ.

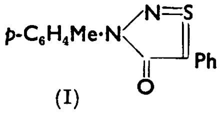
Phenethyl.—It is not always realised that the name phenethyl for $Ph{\cdot}\overset{\beta}{CH_2}{\cdot}\overset{\alpha}{CH_2}$, officially recognized by I.U.P.A.C. (cf. *J.*, 1952, 5096), may be used for substituted derivatives. It is thus correct to write, *e.g.*, 3 : 4-dihydroxyphenethyl (cf. *J.*, 1956, 513) or α-hydroxyphenethyl.

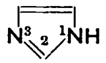
Tropone, Tropylium.—In deference to widespread practice, the name tropone is accepted in place of *cyclo*heptatrienone, and tropylium for the *cyclo*heptatrienyl cation (cf. *J.*, 1956, 2021), though the Editor personally doubts the necessity for such brevity or the ability of these names to express the novel concepts involved. Somewhat analogously, 4-hydroxytropone has been used (*J.*, 1956, 2620) to replace *iso*tropolone (admittedly perhaps an ambiguous description) (*J.*, 1954, 1060). However, as stated in the introduction to this Report, further consideration is required of the nomenclature of this class of compound.

Spirostans.—Final resolution of spirostan nomenclature awaits full proof of the stereochemistry involved. Authors should suit their nomenclature to the structures which they wish to express (cf. *J.*, 1956, 4330).

Quadrivalent Sulphur in Ring Systems.—Names were desired recently (*J.*, 1956, 3189) to express quadrivalent sulphur $=S=$ as a member of a ring system. The "a" nomenclature (aza, thia, etc.) was used in names such as 4-oxo-5-phenyl-3-*p*-tolyl-1-thia(S^{IV})-2 : 3-diazoline for the structure (I).

Methylhistidines.—The glyoxaline (iminazole, imidazole) ring has long and universally been numbered as in (II). Long custom (cf. Mitchell, "British Chemical Nomenclature," Arnold, London, 1948, p. 145) ascribes the numbering as in (III) to histidine, *i.e.*, as if that tautomeric form were the predominant or only one. It is therefore unfortunate that the compound (IV) (a derivative of carnosine) is generally referred to in biochemical literature as 1-methylhistidine, whereas compound (V) (isolated from urine) is there generally termed 3-methylhistidine (cf. *Ann. Reports,* 1955, **52**, 272), *i.e.*, the usual numbering of histidine itself is reversed. Authors in the Society's publications are advised to use the older, recognized histidine numbering, together with formulæ.


(I)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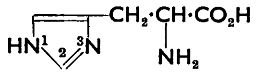
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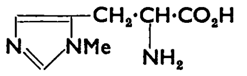

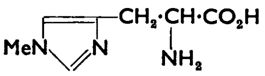
(V)

Demethylene.—This prefix denotes, formally, replacement of CH_2 by two hydrogen atoms. It has been used (*J.*, 1956, 3121) to denote replacement of $-O{\cdot}CH_2{\cdot}O-$ by $-OH\ HO-$ when the complete structure of a molecule was not known.

Stereoisomerism.—Increasing difficulty and improvisation is encountered in designation of various forms of stereoisomerism, in absence of accepted general principles covering modern requirements. For instance, the prefixes *threo* and *erythro* have been borrowed from carbohydrate chemistry for use with hydroxy-aliphatic acids containing the grouping $-CH(OH){\cdot}CH(OH){\cdot}CH_2{\cdot}CH(OH){\cdot}CH(OH)-$ (*J.*, 1956, 1611) and with amino-acids (*J.*, 1956, 1662); *cisoid* and *transoid* have been brought into use for aliphatic isomers each in a special conformation (*J.*, 1956, 2280); the proper use of *exo* and *endo* in polycyclic systems is open to argument in some cases, and definition is often desirable in specific cases (cf., *e.g.*, *J.*, 1956, 2302). For substituted long-chain acids of known absolute configuration, *D* and *L* have had further application (*J.*, 1956, 1620, 2036) with the conventions laid down by Linstead, Lunt, and Weedon (*J.*, 1950, 3333); for alkylamines and related amino-aldehydes of known absolute configuration, (*R*) and (*S*) introduced by Cahn, Ingold, and Prelog (*Experientia*, 1956, **12**, 81) were adopted. The Editor, being personally involved in sponsorship of a particular system for general designation of absolute configuration, would prefer authors to select their own system in this particular respect until some independent authority may rule otherwise.

The use of *d* and *l* in connexion with octahedral groupings (*J.*, 1953, 2675) has continued (*J.*, 1956, 1710).

Desilylation.—The editorial report on nomenclature, 1954, contained suggestions by Dr. J. F. Bunnett for description of reactions in which a group or atom, X, is replaced by another, Y: it was there stated that these suggestions might prove useful but should be used with discretion. Recently (*J.*, 1956, 4859) a brief description was required for replacement of the group $-SiMe_3$ by hydrogen. Strict application of Dr. Bunnett's process would have led to the term protodetrimethylsilylation: this could reasonably be shortened to detrimethylsilylation; but even that appeared too formidable and, instead, the abbreviated " desilylation " was used, though the resulting loss of precision was recognized (desilylation should refer to replacement of any group $-SR_3$ by H, or, strictly, only $-SH_3$ by H).

GENERAL

Concentrations expressed as %.—It should be noted that concentrations expressed simply as " *x*% " apply to % (w/w), *i.e.*, *x* grams of solute in 100 grams of solution. If concentrations are expressed as grams of solute in 100 ml. of solution, they must be specified as " *x*% (w/v)." Other well-recognized forms, such as M, N, *c* (for optical-rotation measurements), may of course be used without explanation; but if other units are chosen they must be clearly specified.

Solvent mixtures for, *e.g.*, chromatography, expressed as ratios, as in " benzene–ether (3 : 2)," are held to refer to relative volumes of the individual solvents used.

" *Personal Communications.*"—Unpublished information from other workers is often acknowledged in the form " A.B.C—, private communication " or " private communication from Dr. A.B.C—." However, " private " communications should not be divulged, and the form " personal communication " is therefore now used in the Society's publications.

Legends for Illustrations.—The Society's printers, in common with most others, now require that legends for illustrations shall form part of the manuscript, and not merely be placed on the diagram itself. Legends are most conveniently handled if typed on a separate sheet (which should be given a page number).

References.—The conventions used in citing references as footnotes were detailed in *Proceedings,* 1955, pp. 78—81 (also available as an offprint). Experience has shown that one change is required. Since the position of Tables and Figures on the final printed pages cannot be guaranteed, difficulty may arise if references cited there for the first time are numbered consecutively with references in the main text. References in Figures and Tables are best cited by letters (italics), being then listed as footnotes immediately below the appropriate Table or Figure; alternatively they can sometimes be given in the parenthetical form which was previously obligatory throughout the *Journal.*

The considerable saving of space achieved when several references to one fact are put together in one group should be noted; and finally attention is drawn again to the details given in *Proceedings* and the need for following them strictly, as well as to the forms of abbreviated titles of journals listed in the January issues of *Current Chemical Papers* and in recent volumes of *Annual Reports.*