EDITORIAL REPORT ON NOMENCLATURE, 1954.*

GENERAL

Ultra-violet and Visible Spectra.—The following decisions were made on May 7th, 1953, by the Publication Committee :

(*a*) For other than pure compounds, curves or parts thereof should not be printed if the requisite facts can be stated in the text. These recommendations exclude, for example, the publication of curves relating to the qualitative identification of substances or groups in impure material and the quantitative determination of substances in mixtures. In exceptional cases the relevant portions of curves may be printed.

(*b*) If the facts can be stated in the text, curves used to establish the identity (or otherwise) of two substances do not require publication (except in special cases).

(*c*) For pure compounds it is permissible to publish visible or ultra-violet absorption curves provided that the following conditions are fulfilled : (i) the purity is reasonably established, (ii) the method of measurement and the range of spectra are adequate, and (iii) the results cannot be adequately presented in numerical form.

(*d*) In most cases, wave-lengths of maxima and minima and extinction coefficients should be given in numerical form, and the scale on which curves are reproduced should be no more than that required to show the general form. For some considerable time many curves reproduced in the *Journal*, without the numerical data, have been larger than needed to show the general form but inadequate for reading off of the numerical data.

(*e*) Visible and ultra-violet spectra should be plotted with long wave-lengths or low frequency on the right, and with ε (E/cd), $E^{1\%}_{1\,\mathrm{cm.}}$, or logarithms to the base 10 of these quantities, increasing upwards.

(*f*) Except in special cases, curves for pure substances should cover the whole range of the instrument used or the whole of the region where absorption occurs, whichever is the less.

Note : Rules for the publication of infra-red spectra are given in *J.*, 1952, 5063. The deposition scheme is confined to infra-red spectra.

References.—Attention is drawn to the abbreviations of journal titles published in *Current Chemical Papers*, January, 1955. These differ in a few cases from those given in the brochure " Presentation of Papers for the Journal of the Chemical Society." The new abbreviations supersede those given in the brochure also for other publications of the Chemical Society (except that the use of *J. Chem. Soc.* is restricted to *Current Chemical Papers*).

Exponential Terms.—Smaller type is always used for superscripts and subscripts than for the main text, and the range of type available for machine-setting of superscripts and subscripts is limited. Thus both for legibility and for ease of setting, the use of complex superscripts and subscripts should be kept to a minimum. This applies particularly to complex exponential terms, where " exp " followed by the term written on the line is always preferable to " e " followed by a complex superscript. *E.g.*, $\exp(-\Delta F_a/\boldsymbol{R}T)$, not $\mathrm{e}^{-\Delta F_a/\boldsymbol{R}T}$. Even in simpler cases, exp is often preferable, *e.g.* $\exp(-\varepsilon_0/\boldsymbol{k}T)$, not $\mathrm{e}^{-\varepsilon_0/\boldsymbol{k}T}$ so as to avoid the subscript to the superscript.

Printing of Mathematics.—Desiderata in the presentation of mathematics are recorded, together with the house rules of the Oxford University Press, in " The Printing of Mathematics," by T. W. Chaundy, P. R. Barrett, and C. Batey, Oxford Univ. Press, 1954. In general, the instructions and information there given apply also to the Chemical Society's publications; however, in the latter, all mathematical operators (d, e, exp, lim, etc.) are without exception printed in roman type, following the Report of the Symbols Committee of the Royal Society, 1951.

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* Reprints of this Report, and of those for 1950, 1951, 1952, and 1953, may be obtained from the General Secretary, The Chemical Society, price 1*s*. each (post free).

PHYSICAL

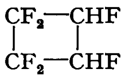
Orbital and Bond Notation.—A new type of bond, designated as a " *schedo*-σ-bond " has been discussed (*J.*, **1954**, 334). In the same paper the different orbital notations of Eyring *et al.* and of Pauling and Wilson are correlated.

ORGANIC

Hydrogen Transfer.—Reactions in which covalently bonded hydrogen changes its site of attachment, either inter- or intra-molecularly, have been designated by the general term " hydrogen transfer " (*J.*, **1954**, 3544).

Hydroethylenic.—The term " hydroethylenic " has been used (*J.*, **1954**, 3569) with reference to a saturated aliphatic system which is particularly prone to conversion into an ethylenic system, *e.g.*, dehydrogenation of dibenzyl to stilbene. This term should be used with caution and only when the concept which it conveys is relevant.

Use of " H."—(*a*) The Editorial Report on Nomenclature, 1952 (*J.*, **1952**, 5059), gave details of the suggested use of *H* to designate the positions of hydrogen in almost completely halogenated organic compounds. This has found application (*J.*, **1954**, 1177) in the names 1*H* : 2*H*-hexafluoro*cyclo*butane (I), 1*H*-pentafluoro*cyclo*butene (II), and 3*H*-pentafluoro*cyclo*butene (III).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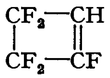
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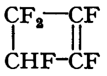
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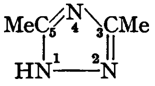
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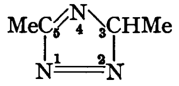
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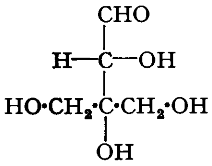
(*b*) The Commission of Nomenclature of Organic Chemistry of I.U.P.A.C. has for some years had under consideration the use of *H* to designate the position of " extra " hydrogen (or, as I.U.P.A.C. prefer to call it, " indicated " hydrogen). Whilst the final rules are still not agreed, the general simple principle is clear. It finds expression in such names as 3 : 5-dimethyl-1*H*-1 : 2 : 4-triazole (IV) and 3 : 5-dimethyl-3*H*-1 : 2 : 4-triazole (V) to distinguish the two forms (cf. *J.*, **1954**, 141).

Apiose.—The stereochemistry of this carbohydrate (*aldo*-D-form = VI) (*J.*, **1954**, 3702), as well as of cordycepose (*J.*, **1951**, 2299, 2301), does not come within the scope of the nomenclature agreed between the American and the British Chemical Societies (*J.*, **1952**, 5108) : furanose-ring formation, *e.g.*, to (VII) involves creation of an asymmetric atom bearing a higher number than that responsible for the original D-prefix. A tentative new nomenclature was used (see *J.*, **1954**, 3704 for details) pending Anglo-American discussion of branched-chain sugars in general.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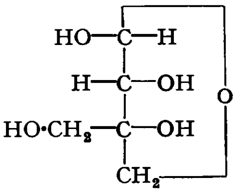
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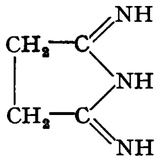

(VIII)

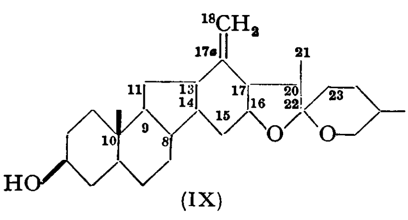
Cyclic Imidines.—Pinner's name (*Ber.*, 1883, **16**, 352), succinimidine, for the compound (VIII), was used in Beilstein's Handbuch, 4th Edn., together with glutarimidine for the next higher homologue (Pinner, *Ber.*, 1890, **23**, 2942); this has been continued by Linstead's school (*e.g.*, *J.*, **1954**, 442). By analogy 1 : 3-di-imino*iso*indoline would become phthalimidine, but that name is used by *Chemical Abstracts* in a different sense, *viz.*, for 1-oxo*iso*indoline. Linstead and his colleagues cite in favour of their use of the imidine names that the generic term imidine ignores the question of fine structure of these potentially tautomeric compounds.

Terpenes.—A detailed report on the nomenclature of terpenes is given in *Chem. Eng. News*, 1954, **32**, 1795. The proposals there made are recommended for use in the Chemical Society's publications.

Steroids.—Experts will recognise that recent developments concerning the stereochemistry at positions 20 and 25 necessitate revision of a few points of steroid nomenclature (*J.*, **1951**, 3526). Such revision must, however, await full clarification of the chemistry.

Conversion of ring C into a five-membered ring and of ring D into a six-membered ring gives compounds of increasing importance. No generally recognised trivial names for such compounds yet exist; but it would seem reasonable, if names are essential, to adopt the proposal (*J.*, 1954, 1740) to call, *e.g.*, (IX) 3β-hydroxy-C-nor-D-homo-5α : 22*a*-spirost-17*a*-en.

Triterpenes.—Some complex nomenclature is exemplified (*J.*, 1954, 1914) by the name 30-nor-19α(H)-taraxastan-20-one for the compound (X). The prefix 30-nor refers to loss of the carbon atom numbered 30 (cf. XI), in accordance with steroid custom (cf. *J.*, 1951, 3534, rule 6·1). The prefix 19α(H) denotes the α-configuration of the hydrogen atom at position 19; this aspect of the stereochemistry might equally have been rendered 19β(Me), for there are as yet no agreed rules as to whether the H or the Me shall govern the prefix.



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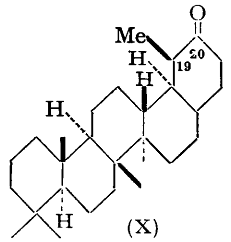

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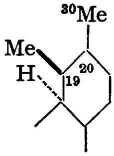


(XI)

Ferrimyoglobin.—The symbolism $MbFe^{2+},H_2O$ for ferromyoglobin, $MbFe^{3+},H_2O$ for ferrimyoglobin, and $MbFe(II)O^{2+}$ for oxymyoglobin has been adopted (*J.*, 1954, 3142). The superscripts 2+ and 3+ denote that the iron is ionically bound, the sixth co-ordination position being occupied by a water molecule; the symbol (II) indicates a covalently bound complex of ferrous iron. MbFe(IV) denotes the higher valency state containing covalently bound iron, but of uncertain structure.

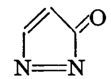
Triaryl Phosphite Dihalides.—This designation has been used (*J.*, 1954, 2281) for compounds $(ArO)_3PHal_2$, with the note that the systematic names (cf. *J.*, 1952, 5122) would be triaryloxyhalogenophosphonium halides if the compounds are electrovalent, or triaryl dihalogenophosphoranetrioates if covalent.

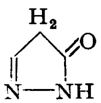
Azoxy-compounds.—Unambiguous nomenclature was needed (*J.*, 1954, 4069) for asymmetric azoxy-compounds $R\cdot N{:}N(O)\cdot R'$. The compound R′H [where R′ is the residue attached to the N(O) group] was regarded as the parent compound, into which the $R\cdot N{:}N(O)$-group was substituted. In conformity with the I.U.P.A.C. name phenylazo (not benzeneazo) for $Ph\cdot N{:}N$- (see *J.*, 1952, 5062, 5098), the $R\cdot N{:}N(O)$-groups were termed arylazoxy (not areneazoxy) or alkylazoxy (not alkaneazoxy). Arylazoxy- and alkylazoxy-groups, being treated as substituents into the compound R′H, must be listed alphabetically with any other substituents in the R′ moiety. The following examples illustrate the method :

$CH_3\cdot N{:}N(O)\cdot CHMe_2$	2-(Methylazoxy)propane
$PhEtCH\cdot N{:}N(O)\cdot CHMe_2$	2-(1-Phenylpropylazoxy)propane
$Ph\cdot CH_2\cdot N{:}N(O)\cdot C_6H_4Cl$-*p*	*p*-(Benzylazoxy)chlorobenzene
p-$C_6H_4Cl\cdot CH_2\cdot N{:}N(O)\cdot Ph$	(4-Chlorobenzylazoxy)benzene
p-$C_6H_4Cl\cdot N{:}N(O)\cdot CH_2Ph$	ω-(*p*-Chlorophenylazoxy)toluene
$Ph\cdot N{:}N(O)\cdot CH_2\cdot C_6H_4Cl$-*p*	*p*-Chloro-ω-(phenylazoxy)toluene
p-$C_6H_4Br\cdot N{:}N(O)\cdot CH_2\cdot C_6H_4Cl$-*p*	ω-(*p*-Bromophenylazoxy)-*p*-chlorotoluene
p-$C_6H_4Br\cdot N{:}N(O)\cdot CH_2\cdot C_6H_4Br$-*p*	*p*-Bromo-ω-(*p*-bromophenylazoxy)toluene

Parentheses were used freely, particularly when it was necessary to avoid confusion with the trivial names for symmetrical azoxy-compounds, such as azoxybenzene for $C_6H_5\cdot N{:}N(O)\cdot C_6H_5$, or with cases where the position of the azoxy-oxygen atom is not known.

(XIII)





(XIV)

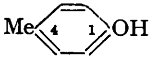
Cyclic Ketones.—A regrettable error occurred in last year's Editorial Report on Nomenclature. The name pyrazolone was ascribed (*J.*, 1953, 4204) to the compound (XIII); this should indeed be the systematic name for that compound, but that name has long been used for the dihydro-derivative of which one form is (XIV). The main argument developed in the Report is unaltered, and this older usage merely further complicates the position. It is hoped that I.U.P.A.C. will shortly consider this and related problems, so a fuller discussion is reserved.

Ethers of Natural Products.—Ethers of many natural products have generally been designated by unqualified alkyl prefixes. Such practice was exemplified by 2-methyl glucose or 2-methylglucose, but the carbohydrate nomenclature has now fallen into line with general chemical nomenclature, this substance now being termed 2-*O*-methylglucose (cf. *J.*, 1952, 5108), in distinction from the *C*-alkyl derivatives. Analogous use of unqualified alkyl prefixes has been common also with other natural products, notably pyrylium salts, flavones, and certain alkaloids. The *O*-prefix has however been used recently also in such cases, *e.g.*, *O*-ethyl*neo*quassin (*J.*, 1954, 4238), hexa-*O*-methyldistemonanthin (*J.*, 1954, 4594), and general adoption of this system is highly desirable.

The *O*-prefix is of course not needed when the compounds are named by the ether terminology, *e.g.*, glucose 2-methyl ether, *neo*quassin ethyl ether, distemonanthin hexamethyl ether, since the word " ether " denotes linkage to oxygen. Equally the term ether should not be used to denote other types of linkage, *e.g.*, through nitrogen or sulphur.

Use of o-, m-, *and* p-*Prefixes.*—It was stated earlier (*J.*, 1952, 5063) that use of *o*-, *m*-, and *p*- should be confined to chemical names, and that in phrases such as *ortho*-effect, *ortho*-substituent, *meta*-directing, *para*-group the prefix should be written in full. It is, however, desirable to restrict the use of the single-letter forms even in chemical names to simple compounds, for any slight complexity tends to render them obscure. They should be restricted to cases of three types: (i) disubstitution of a single benzene nucleus, *e.g.*, *p*-dichlorobenzene, *p*-bromonitrobenzene; (ii) monosubstitution in a phenyl radical, *e.g.*, 1-*p*-chlorophenylnaphthalene, 1 : 1-di-*p*-chlorophenylethane, di-*p*-chlorophenyl sulphide; and (iii) monosubstitution in a substituted benzene derivative having a trivial name, *e.g.*, *o*-nitroaniline, *p*-chlorotoluene, *m*-bromoanisole, *m*-nitrobenzoic acid, 4-bromo-*m*-xylene (or 1-bromo-2 : 4-dimethylbenzene). Numerals should be used in all other cases, *e.g.*, 4 : 4′-dinitrodiphenyl, 4-aminodibenzyl, 1-4′-nitrobenzylnaphthalene. Xylenols, xylidines, etc., are best called 3 : 5 : 1-xylenol, 2 : 4 : 1-xylidine, etc. (cf. next paragraph).

Methyl-substituted Derivatives of Benzene.—It appears necessary to call attention again to abandonment by the Chemical Society of its practice of giving the lowest number(s) to methyl in simple methyl-substituted benzene derivatives such as the cresols, xylenols, toluidines, xylidines, toluic acids. In all such cases, in accordance with I.U.P.A.C. rules (*J.*, 1952, 5073, footnote 22), the functional group (OH, NH_2, CO_2H) carries the number 1, as in (XV), (XVI), and (XVII). Similarly in the tolyl and the xylyl radical the point of attachment carries the number 1, as in (XVIII).



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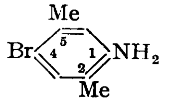

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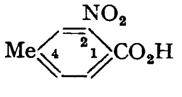

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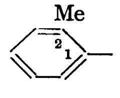


(XVIII)

Systematic Names for Substitution Reactions.—The following suggestions by Dr. J. F. Bunnett (University of North Carolina) were printed in Dr. A. M. Patterson's column in *Chem. Eng. News*, 1954, **32**, 4019, and are reprinted below by kind permission. The proposals lead to some curious and occasionally cumbrous names, and so should be used with discretion; but they provide a logical system of wide applicability for saying a lot intelligibly in a short space, and authors may like to make use of them. The article reads:

In the very extensive and very useful work on systematic nomenclature in organic chemistry, most attention has been devoted to the naming of *compounds*. The present proposal relates to another aspect of the organic chemist's language, the naming of *reactions*. Little attention has been paid to systematic nomenclature for reactions, in part because the principal motivation for systematic nomenclature has come from indexers, and indexers in general have not shown the same interest in the thorough and systematic indexing of reactions that they have shown in the indexing of compounds. In consequence, one can locate information on a compound in the literature relatively quickly and easily, whereas locating a certain type of reaction through the usual indexes is often next to hopeless. It seems possible that part of the comparative disinterest of indexers in reactions stems from the lack of definite, agreed-upon names for reactions.

Quite apart from the matter of indexing the literature, there is need for systematic names for reactions for use in discussions both of synthetic organic chemistry and of reaction mechanisms.

In practice today, the chemist often finds himself designating a reaction by the name of its discoverer or using a wordy phrase or clause to denote a chemically simple process. The former practice puts an enormous tax on the memory and is often ambiguous (*e.g.*, the Hofmann degradation), while the latter contributes both bulk and obscurity to the discussion. The present proposal relates only to substitution reactions, though need for systematic names for other types of reactions is obvious.

For some substitution reactions, mainly reactions in which hydrogen is displaced, chemists have simple, straightforward names which convey a definite meaning usually without ambiguity; for example, " nitration," " amination," " *iso*propylation," and " chlorosulphonation." However, for many substitutions, especially those in which a group other than hydrogen is displaced, there are no straightforward names; for example, the reaction of *p*-chloronitrobenzene with sodium methoxide to form *p*-nitroanisole would ordinarily be referred to as " displacement of chlorine by methoxide." This phrase can perhaps be tolerated in a discussion of preparative chemistry, but in a discussion of reaction mechanisms or reactivity in which the above reaction is compared with others such as " the reaction of aryl halides with piperidine " and " the cleavage of aryl quaternary ammonium salts by alkoxide ions," the use of such phrases introduces both bulk and confusion of thought. The situation is perhaps even worse in describing electrophilic substitution of groups other than hydrogen; thus one must speak of " the anomalous displacement of bromine during nitration."

I therefore propose a concise general method for naming substitution reactions. The name is composed of these parts: the name of the incoming group, the syllable " de," the name of the departing group, and the suffix " ation." For euphony, suitable elision of vowels or introduction of consonants is occasionally necessary. For example, the name of the reaction in which chlorine is displaced by methoxide is composed of the parts: *methoxy* + *de* + *chloro* + *ation*. These are fused with introduction of " in " for " o " (to accord with general chemical usage) to form the name: *methoxydechlorination*. The reaction of aryl bromides with piperidine[1] is named " piperidinodebromination." The reaction of acetate ion with an alkyl bromide to form an acetate ester becomes " acetoxydebromination." It should be noted that these names are based only on the structures of the starting materials and the products, and do not imply a knowledge of mechanism. Further, they do not mention the nature of the site of substitution. The chemist who might wish to specify such further information can do so, however, by the use of suitable adjectives or modifying phrases; thus, one might write of " nucleophilic aliphatic iododechlorination " or " electrophilic aromatic nitrodebromination."

In regard to reactions involving displacement or introduction of hydrogen, it is proposed that the group be described as " proto." This is to avoid confusion with the firmly established terms " dehydration " and " dehydrogenation," both of which have a meaning different from that intended here. Thus one would have " nitrodeprotonation " for ordinary nitration, and " protodesulphonation " for the cleavage of sulphonic acids by mineral acids. If another isotope of hydrogen is involved, the group should be named " deutero " or " tritio." Thus, " deuterodeprotonation " during exchange of deuterium and protium, and " bromodetritiation " for displacement of tritium during bromination.

It is not proposed or imagined that these names should replace common expressions such as " the nitration of toluene " or " the Friedel and Crafts *iso*propylation of benzene " in ordinary chemical discourse. However, they will be most useful in discussing the nitration of 1 : 4-di*iso*propylbenzene in which either a hydrogen may be replaced, forming 2-nitro-1 : 4-di*iso*propylbenzene, or an *iso*propyl group may be displaced, forming 4-nitro*iso*propylbenzene;[2] the two reactions concerned are " nitrodeprotonation " and " nitrode*iso*propylation." Systematic names for substitution processes will also be of great use in considering processes such as the sulphonation of benzene-*t*, in which reaction the rates of " sulphodeprotonation " and " sulphodetritiation " are not equal.[3] They will also be of great use in indexing.

Literature Cited:

[1] E. Berliner and L. C. Monack, *J. Amer. Chem. Soc.*, 1952, **74**, 1574.

[2] D. V. Nightingale, *Chem. Rev.*, 1947, **40**, 117; she describes scores of reactions to which this new terminology can be profitably applied.

[3] D. Melander, *Arkiv Kemi*, 1950, **2**, 211.

BIOCHEMISTRY

The Commission of Nomenclature of Biological Chemistry of I.U.P.A.C. has issued the following " New Supplementary Rules for the Nomenclature of Vitamins " (*Compt. rend.* 17th Conference I.U.P.A.C., 1953, pp. 149—150) :

A. *Fat-soluble vitamins* :

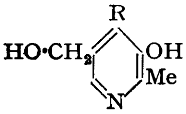
Rule 4. (*a*) When 2-methyl-3-phytyl-1 : 4-naphthaquinone is designated by a trivial name, *e.g.*, in biochemical papers, that name shall be phylloquinone.

(*b*) When 2-difarnesyl-3-methyl-1 : 4-naphthaquinone is designated by a trivial name, *e.g.*, in biochemical papers, that name shall be farnoquinone.

B. *Water-soluble vitamins.*

Rule 5. (*c*) The term pyridoxine may be used as a group name to designate the naturally occurring pyridine derivatives with vitamin B_6 activity.

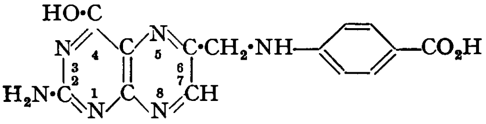
Derivatives of 3-hydroxy-5-hydroxymethyl-2 : 4-dimethylpyridine in which one of the functional groups designated below is attached to, or replaces, the 4-methyl group shall be named : pyridoxol ($CH_2{\cdot}OH$ at position 4) ; pyridoxal (CHO at position 4) ; pyridoxamine ($CH_2{\cdot}NH_2$ at position 4).



$R = CH_2{\cdot}OH$ pyridoxol
$R = CHO$ pyridoxal
$R = CH_2{\cdot}NH_2$ pyridoxamine

Rule 7. Until the nomenclature of the *cyclo*hexitols is codified, the substance usually designated *meso*inositol should continue to be called *meso*inositol.

Rule 9. (*a*) The name pteroic acid shall designate the compound formed by linkage of $C_{(6)}$ of 2-amino-4-hydroxypteridine by means of a methylene group with the nitrogen atom of *p*-aminobenzoic acid.



(*b*) The pteroylglutamic acids may be designated generically as folic acids.

(*c*) The pure substance hitherto known as folic acid, folacine, or vitamin B_c shall be named pteroylmonoglutamic acid.

(*d*) Compounds analogous to pteroylmonoglutamic acid but containing several glutamic acid residues united by amide linkages may be named pteroyltriglutamic acid, pteroylheptaglutamic acid, etc.