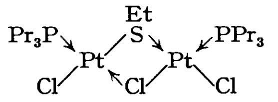
EDITORIAL REPORT ON NOMENCLATURE, 1953.*

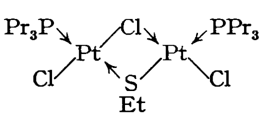
INORGANIC

Ions.—When discussing the conversion of the octahedral ion $[\mathrm{Co\,en_2Cl_2}]^+$ into $[\mathrm{Co\,en_2ClX}]^+$ it was necessary to discuss intermediate formation of the optically inactive ion $[\mathrm{Co\,en_2Cl}]^{++}$. The term "cobaltium ion" was used for the intermediate containing quinquecovalent cobalt (*J.*, 1952, 2696), "for temporary convenience"; analogy was with "carbonium," the name applied to what is left when a maximally covalent form of carbon, CR_4, loses one ligand R with its bonding electron. The qualifying phrase signified that this nomenclature was subject to revision, inasmuch as attention must shortly be paid to the nomenclature of ions in general.

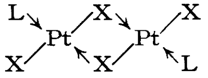
Bridged Complexes.—The structures (I) and (II) required differentiation (*J.*, 1952, 2363).

(I)

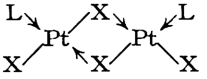




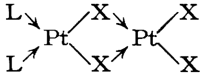
(II)



(III)
trans-symmetrical



(IV)
cis-symmetrical



(V)
unsymmetrical

This was done by extending the nomenclature used for (III)—(V), so that (I) was named *cis*-PSP-*cis*-symmetrical-dichlorobistri-*n*-propylphosphine-μ-chloro-μ′-ethylthioplatinum, and (II) became the *cis*-PClP compound.

Asymmetry of Octahedral Compounds.—Optical activity among octahedral compounds requires great care in assignment of prefixes. The footnotes in *J.*, 1952, 2674, 2676, should be studied; it has been necessary in some cases to use Werner's prefixes *d*, *l*, and in others *D*, *L*.

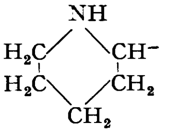
I.U.P.A.C.—Recommendations for inorganic nomenclature are in preparation by I.U.P.A.C. but have not yet been published. Until publication occurs, action on many matters of conflicting usage is deferred.

ORGANIC

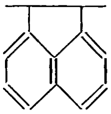
I.U.P.A.C.—In last year's Editorial Nomenclature Report the following corrections should be made:

p. 5087. The statement "$\mathrm{MeO{\cdot}PO_2{\cdot}O{-}}$ is methoxyphosphoryloxy" should be deleted (such a radical would have sexavalent phosphorus).

p. 5094. Formula of 2-piperidyl to be



p. 5096. Formula of 1 : 6-acenaphthenylene to be



p. 5120. $\mathrm{CH_2{\cdot}OH}$ to replace H on $C_{(5)}$ of the right-hand ring of the second formula.

p. 5130. Phosphenimidic chloride to be $\mathrm{Cl{\cdot}P(O){:}NH}$.

The changes called for by the I.U.P.A.C. rules reprinted in the last Report have been introduced gradually in the *Journal* during 1953; they will come into regular use in 1954.

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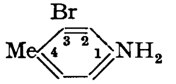
* Reprints of this Report, and of those for 1950, 1951, and 1952, may be obtained from the General Secretary, The Chemical Society, price 1*s.* each (post free).

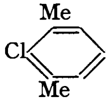
Emphasis may again be laid on the change of the prefix for $=O$ from keto to oxo in names of specific compounds, and of that for CO_2Alk from carbalkoxy to alkoxycarbonyl, etc.

Attention is also drawn to the following points :

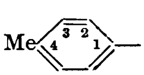
(i) In methyl-substituted benzene derivatives containing functional groups the number 1



(VI)



(VII)



(VIII)

will be assigned to the functional group, and not to a methyl group as hitherto. Thus, (VI) is 3-bromo-4-methylaniline or 3-bromo-*p*-toluidine, (VII) is 4-chloro-3 : 5-dimethylphenol or 4-chloro-3 : 5 : 1-xylenol. Radicals are numbered similarly, as in *p*-tolyl (VIII), with the methyl group as 4 (*J.*, 1952, 5091, footnote 22).

(ii) Acid radicals end in " oyl," except formyl, acetyl, propionyl, butyryl, *iso*butyryl, valeryl, *iso*valeryl, oxalyl, malonyl, succinyl, glutaryl (*i.e.*, aliphatic acids up to C_5) (*J.*, 1952, 5075, rule 58.3), and the α-monoradicals aspartyl $HO_2C{\cdot}CH_2{\cdot}CH(NH_2){\cdot}CO{-}$ and glutamyl $HO_2C{\cdot}CH_2{\cdot}CH_2{\cdot}CH(NH_2){\cdot}CO{-}$ (*J.*, 1952, 5079).

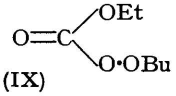
(iii) Pentyl replaces amyl (*J.*, 1952, 5073, rule 54.1).

(iv) The *iso*-nomenclature to indicate terminal branching of an aliphatic chain is permitted only up to C_6, and then only for the unsubstituted radicals (*J.*, 1952, 5073, rule 54.2).

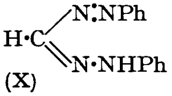
(v) The numbering rules, though not new, are often not fully understood. They are given in I.U.P.A.C. rules 51, 64, and 66, and are discussed in the Editorial notes thereto (*J.*, 1952, 5071, 5076, 5077).

(vi) In all cases the point of attachment of radicals has the lowest possible number. For alkyl and monocyclic hydrocarbon radicals, this is invariably 1. *E.g.*, $CH_3{\cdot}CH_2{\cdot}CH_2{\cdot}CH_2{\cdot}CHMe{-}$ is 1-methylpentyl, not 2-hexyl.

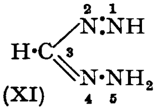
Per-esters.—In certain mixed per-esters it became necessary to differentiate the attachment of the alkyl groups. To achieve this the ester (IX) was named *O*·*O*-butyl *O*-ethyl percarbonate (*J.*, 1953, 1809).



(IX)



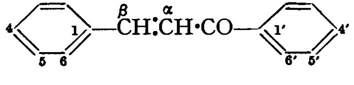
(X)



(XI)

Formazans.—The name formazyl has frequently been applied to the compound (X). This name does not lend itself to ready extension to analogues. The practice of Beilstein's " Handbuch " has therefore been adopted, of naming the parent (XI) formazan, with numbering as shown. The substance (X) (formazyl) thus becomes 1 : 5-diphenylformazan (*J.*, 1953, 3538, 3881).

Chalkones (*Phenyl Styryl Ketones*).—In the past there have been inconsistencies in choice of the ring to be distinguished by primed numerals (cf. *J.*, 1953, 2185, the styryl ring; *J.*, 1951, 569, the ring adjacent to the keto-group). Henceforth the numbering of chalkone should be as in (XII); this is consistent with *Chem. Abs.* usage (*Chem. Abs.*, 1945, **39**, 5931) and Beilstein's " Handbuch."



(XII)

Stereochemistry.—(*a*) A particular case of conflict between the amino-acid and the carbohydrate usage of D and L is provided by adrenaline and noradrenaline (*J.*, 1953, 3324), but without an agreed solution.

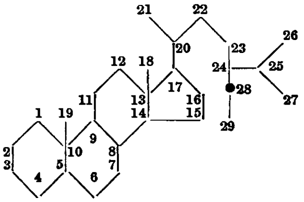
(*b*) Four international authorities jointly recommend replacement of polar (in the stereochemical sense) by axial (*Nature*, 1953, **172**, 1096). Use of the terms equatorial and axial will therefore be encouraged in the Society's publications; it is hoped that all authors will concur in the need for common practice.

(*c*) The steroid use of α and β has been applied in the tropine field (*J.*, 1953, 721).

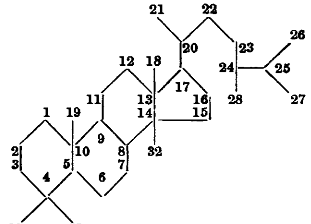
(*d*) Several authors prefer the use of heavy (bold) bonds to that of ordinary bonds in steroid formulæ (*e.g.*, *J.*, 1953, 2916), as is common practice in terpene chemistry. The CIBA rule 2 (*J.*, 1951, 3527) merely prescribes that a "full line" shall be used to denote β-configuration; use of the heavy full line seems useful and will be encouraged.

(*e*) A special symbolism has been used to denote the steric relation of hydroxyl groups in a zig-zag carbohydrate chain (*J.*, 1953, 984).

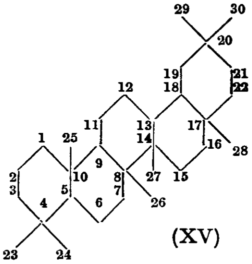
Triterpenes.—Triterpene formulæ are now written so as to correspond with those of steroids (cf. *J.*, 1952, 5060). Numbering has also been changed to correspond broadly with that in the steroid series (*J.*, 1953, 1419) and is exemplified by stigmastane (XIII), eburicane (XIV; number 29 is omitted) (*J.*, 1953, 2553, 3021; contrast p. 2169), and oleanane (XV) (rings A, B, & C) (*J.*, 1953, 3025). When these examples are compared with one another and with abietane (XVI) (phenanthrene numbering) (*J.*, 1953, 3073), and the unequal treatment of methyl groups is noted, it is apparent that finality has not necessarily been reached.



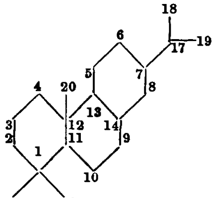
(XIII)



(XIV)



(XV)



(XVI)

Relay.—When, in a long synthesis, an intermediate is prepared by complete synthesis in small quantity, and further supplies are drawn from natural sources or are derived from natural products, that intermediate may be described as a relay (*J.*, 1953, 361). The word relay should be restricted to that sense.

Isotopically Labelled Compounds.—Mention was made (*J.*, 1951, 3516; 1952, 5061) of proposals made jointly by the Editorial Board of the Biochemical Society and the Editors of the Chemical Society, and some examples were then given. These proposals received extensive test in an article in *Quarterly Reviews* (1953, **7**, 407) where they were applied to 150 individual compounds; except that a slight extension was needed in one direction, no difficulties were met. We therefore reprint the nomenclature details given in that article (methods of extending the scheme to cover quantitative aspects may be obtained from the Editor):

The symbol for the isotope introduced is placed in square brackets directly attached to the front of the name, as in [^{14}C]urea.

When more than one position in a substance is labelled by means of the same isotope the number of labelled atoms is added as a right-hand subscript (cf. ordinary formulæ), as in [$^{14}C_2$]glycollic acid.

When isotopes of more than one element are introduced, their symbols are arranged in alphabetical order, including ^{2}H and ^{3}H for deuterium and tritium respectively.

The isotopic prefix precedes that part of the name to which it refers, as in 2-acetamido-7-[^{131}I]iodofluorene, α-naphth[^{3}H]oic acid ($C_{10}H_7{\cdot}CO_2{}^3H$), sodium [^{14}C]formate, 1-amino[^{14}C]-methyl*cyclo*pentanol ($NH_2{\cdot}{}^{14}CH_2{\cdot}C_5H_8{\cdot}OH$).

When not sufficiently distinguished by the foregoing means, the positions of isotopic labelling are indicated by Arabic numerals, Greek letters, or prefixes (asap propriate), placed within the square brackets and before the symbol of the element concerned, to which they are attached by a hyphen; examples are [1-$^2H_1$]ethanol ($CH_3{\cdot}CH^2H{\cdot}OH$), [1-^{14}C]aniline, [α-^{14}C]-leucine, [*carboxy*-^{14}C]leucine, [*Me*-^{14}C]*iso*leucine, [6 : 7-$^{14}C_2$]xanthopterin, [αβ-$^{14}C_2$]maleic anhydride, [1-^{14}C : ^{13}2-C]acetaldehyde, [βγ-$^{13}C_2$: ^{34}S]methionine, [β-^{14}C : αβ-$^2H_2$: ^{15}N]serine.

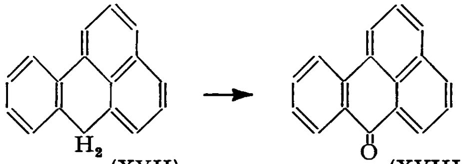
When the position of isotopic labelling is indeterminate, the possible positions are specified together with the number of atoms which are labelled, as in [*ar*-$^{14}C_1$]benzaldehyde (one ^{14}C in the benzene ring), [4 : 6-$^{14}C_1$]adenine (one ^{14}C, at position 4 or 6), D-[1 : 6-$^{14}C_1$]fructose (one ^{14}C, at position 1 or 6). (The device illustrated in the last two examples is an extension of the " editorial " proposals.)

Carbinol.—It was stated in the Report for 1952 (*J.*, 1952, 5061) that use of the term carbinol was very rarely justified in the light of modern nomenclature and should be restricted to *series* of compounds $CRR'R''{\cdot}OH$. The Editors are indebted to the Manchester school for pointing out one further context in which carbinol can be usefully employed in non-specific nomenclature, namely, when it is desired to show that a particular group is directly attached to a $C{\cdot}OH$ unit. Thus, an acetylenic carbinol denotes a compound containing the grouping $C{\equiv}C{\cdot}C{\cdot}OH$, and this name differentiates it from a compound containing, *e.g.*, $C{\equiv}C{\cdot}C{\cdot}C{\cdot}OH$ where the $C{\equiv}C$ and the $C{\cdot}OH$ units are separated by other atoms. In all cases, however, the names for specific compounds should normally be on orthodox lines and not on the carbinol convention.

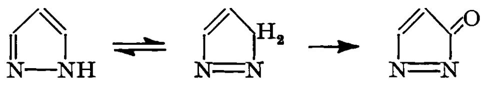
Bis.—The prefix bis has often been used in the *Journal* in order (*a*) to obviate conjunction of two di's, as in bisdinitrophenylhydrazone or 1 : 4-bis-*p*-diphenylylpiperazine (*J.*, 1953, 1941), and (*b*) to indicate two complex groups in contradistinction from simple substitution. The second purpose needs some explanation and also some warning.

As simple illustrations, dichloroacetylbenzene is $C_6H_5{\cdot}CO{\cdot}CHCl_2$, but bischloroacetylbenzene is $C_6H_4(CO{\cdot}CH_2Cl)_2$; dimethylaminophenanthrene is $C_{14}H_9{\cdot}NMe_2$, bismethylaminophenanthrene is $C_{14}H_8(NHMe)_2$; dichloromethylamine is $CHCl_2{\cdot}NH_2$ bischloromethylamine is $(CH_2Cl)_2NH$. This usage on occasions requires care : thus bismethylaminomethylphenanthrene is ambiguous as it might refer to $C_{14}H_8(CH_2{\cdot}NHMe)_2$ or to $C_{14}H_9{\cdot}CH(NHMe)_2$. Further, I.U.P.A.C. rules 49 and 50 (*J.*, 1952, 5071) do not mention bis. Indeed, rule 50 states that in cases of ambiguity parentheses may be used; and the preceding bis-compounds may be unambiguously named di(chloroacetyl)benzene, di(chloromethyl)amine, di(methylamino)methylphenanthrene, and di(methylaminomethyl)phenanthrene. Use of bis in this sense is rare in literature other than that of Great Britain, and its limitations make its international adoption doubtful. Its use should be restricted to simple unambiguous cases; generally it may be replaced by judicious use of parentheses.

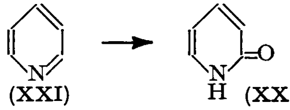
Cyclic Ketones.—Certain cyclic compounds can be, formally, converted into ketones by simple replacement of CH_2 by CO; *e.g.*, *meso*benzanthrene (XVII) ⟶ *meso*benzanthrone (XVIII); pyrazole (XIX*a*, *b*) ⟶ pyrazolone (XX). In such cases the termination of the name may be simply changed to -one. By custom, this termination is sometimes used (particularly but not exclusively for heterocyclic ketones) when, formally, oxygen is added without replacement; *e.g.*, pyridine C_5H_5N (XXI) gives 2-pyridone, C_5H_5ON (XXII); similarly, phenanthrone is sometimes used. This leads to difficulty with reduced compounds : thus, the ketone (XXIII) is the dihydro-derivative of (XXII) and so should be named dihydro-2-pyridone : on the other hand it is the ketone formed by replacement of CH_2 by CO in tetrahydropyridine and so should be named tetrahydropyridone. Since this argument cannot be resolved, neither name should be used, but (XXIII) should be called 1 : 2 : 3 : 4-tetrahydro-2-oxopyridine.



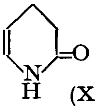
(XVII) (XVIII)



(XIX*a*) (XIX*b*) (XX)



(XXI) (XXII)



(XXIII)

The termination -one should be restricted to simple unambiguous cases of formal replacement of CH_2 by CO, and to the long-established pyridone, quinolone, and *iso*quinolone in their unreduced forms.

Typographical.—The Society's printers set formulæ by use of pieces of type which can reproduce bonds vertically, horizontally, or at 45°, but not at other angles. If the more costly blocks are to be avoided, formulæ should be drawn by using bonds only in these directions. Ingenuity is often called for; examples of "awkward" formulæ satisfactorily reproduced in type can be seen in, *e.g.*, *J.*, 1953, 3125, 3126.

Mixing of formulæ and letter press is a difficult and costly process. This can frequently be avoided by placing Tables under reaction schemes, in cases where physical data require to be attached to formulæ (see *J.*, 1953, 2984—5, 3684).