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Definitive Report of the Committee for the Reform of Nomenclature in Organic Chemistry.

Introduction.

In the domain of organic chemistry, several names can be given to the same compound. This flexibility of nomenclature has the great advantage of facilitating clear expression of thought and the drawing of structural analogies, but is a serious obstacle in the compilation of indexes.

This difficulty was felt as long ago as 1892, and the celebrated Congress of Geneva, at which 34 of the best qualified chemists of 9 European countries created the Geneva nomenclature, endeavoured to overcome it by stating as Rule 1 of its memoir: "Together with the customary name, there shall be given to every organic compound an official name under which it may be found in indexes and dictionaries." As is well known, the intention of the Congress of Geneva has not been realised. The Geneva nomenclature has been sufficiently elaborated only for acyclic compounds, and for many of these, and still more for other compounds, the names resulting from its application are much too complicated. It is probably for this reason that the Commission of 1892 did not complete its work.

An official nomenclature for indexes which was desirable 40 years ago has to-day become unnecessary for the following reasons:

(1) A new edition of Beilstein began to appear in 1918; this admirable work renders bibliographical research extraordinarily easy.

(2) The problem is solved by tables of formulæ, which are now in use in a number of chemical journals and also in Chemical Abstracts and Chemisches Zentralblatt.

In the meantime, the Geneva system of nomenclature has been of very great value to organic chemistry. Its fundamental ideas are of the greatest importance from the systematic point of view throughout organic chemistry. For this reason, the classification in Beilstein is based upon it.

It has already been mentioned that the Geneva names are frequently inconvenient and impracticable for ordinary use. The editors of Beilstein and other works of reference have rightly indexed them together with their common names.

Now a revision of these names has become imperative, for the number of compounds has increased enormously and their discoverers, although adhering as much as possible to custom, have not always been happy in their choice of names and have sometimes even adopted names that are obviously incorrect.

With the object of terminating this unfortunate state of affairs the International Union of Chemistry in 1922, at the suggestion of Sir William Pope, appointed a working committee, selected from the editors of the most important chemical journals, to reform the nomenclature of organic chemistry : Messrs. Crane, Greenaway and Marquis, representing Chemical Abstracts, the Journal of the Chemical Society of London, and Le Bulletin de la Société chimique de France, respectively. This committee was instructed to prepare a report and submit it to the committee of the Union, for approval. In the following year the working committee was enlarged by the inclusion of representatives of Gazzetta chimica (Paternó), Helvetica Chimica Acta (Pictet), and Recueil des travaux chimiques des Pays-Bas (Holleman). The last was elected president, and M. Marquis secretary.

In course of time the working committee underwent the following changes : Mr. Crane was replaced by Mr. Patterson, and Mr. Greenaway (assisted by Professor Gibson) retired, his place being taken by Professor Barger. M. Paternó was soon succeeded by M. Peratoner, who, however, was prevented by illness from taking part in the meetings. After his death, the Italian Chemical Society nominated M. Mario Betti, who took no part in the preparation of the report (see below) but attended the 8th meeting at Warsaw in 1927, the 9th at The Hague (1928), and the 10th at Liége (1930), at which the report was discussed and to some extent modified. Herr Prager, the editor of Beilstein, appointed by the Verband deutscher chemischer Vereine as its representative on the working committee, was also present at Liége.

The working committee met in Paris on several occasions during 1924—28; the result of its work was a report which was presented at The Hague in 1928 to the committee for the reform of the nomenclature of organic chemistry. This committee proposed several modifications, which were considered by the working committee. The amended report was discussed by the committee at the meeting at Liége in 1930 and was unanimously adopted.

It is not the intention of this report to interfere with the systems of nomenclature employed in Beilstein and in Chemical Abstracts : these two publications have for many years adopted their own systems, which are quite similar to the rules now adopted. On the contrary, the object of the committee has been the preservation of common usage as much as possible (see rule 1 below) and its embodiment in print with some simplification and the removal of incorrect names. The committee hopes that the flexible nomenclature thus created will be more and more used by authors of memoirs and of treatises on organic chemistry and also in teaching and that the editors of journals will recommend its use as much as possible.

Rules.

Index: I. General.—II. Hydrocarbons: (1) Saturated; (2) unsaturated; (3) cyclic.—III. Fundamental heterocyclic compounds. —IV. Simple functions.—V. Complex functions.—VI. Radicals.—VII. Numbering.

I. *General.*

1. As little change as possible is to be made in terminology universally accepted.

2. For the present, only the nomenclature of compounds of known constitution will be dealt with, the problem of naming substances of imperfectly known constitution being reserved for later consideration.

3. The precise form of words, endings, etc., prescribed by the rules may be altered by sub-committees to suit the requirements of individual languages.

II. *Hydrocarbons.*

4. The names of saturated hydrocarbons will end in *ane*. Open-chain hydrocarbons will be known generally as *alkanes*.

5. The names methane, ethane, propane and butane are retained for the first four saturated normal hydrocarbons. For those containing more than four atoms of carbon, names derived from Greek or Latin numerals will be used.

6. Branched-chain hydrocarbons are regarded as derivatives of normal hydrocarbons; their names will be determined by the longest chain containing the maximum number of double or triple linkings (preference being given to the double linking where ambiguity arises), or, in the case of saturated hydrocarbons, by the longest chain in the formula. In cases where there might be doubt as to the choice of the longest chain, that one will be selected which admits of the maximum of substitution.

7. In cases where there are several side chains, the order in which these will be named will correspond to their degree of complexity. The chain having the greatest number of secondary and tertiary atoms is to be regarded as the most complex. The alphabetical order may also be followed in such cases.

8. The names of open-chain unsaturated hydrocarbons containing only one double linking will be formed by substituting the termination *ene* for the *ane* of the corresponding saturated hydrocarbons; if there are two double linkings, the termination will be *diene*, and

so on. These hydrocarbons will be known generally as *alkenes, alkadienes, alkatrienes*, etc. Examples : Propene, hexene.

9. The names of hydrocarbons containing the triple linking will end in *yne, diyne*, etc. The class will be known as the *alkynes.* Examples : Propyne, heptyne.

10. If double and triple linkings are both present in the fundamental chain, the terminations *enyne, dienyne*, etc., will be used. The general name of these hydrocarbons will be *alkenynes, alkadienynes*, etc.

11. Saturated monocyclic hydrocarbons will be known generally as cyclo*alkanes* and will take the names of the corresponding saturated open-chain hydrocarbons with the prefix *cyclo.*

12. When they are unsaturated, rules 8—10 will be applied. However, for partly saturated polycyclic aromatic compounds the prefix *hydro*, preceded by *di-*, *tetra-*, etc., will be used. Example : Dihydroanthracene.

13. Aromatic hydrocarbons will be denoted by the termination *ene* and will otherwise retain their customary names. The name *phene*, however, may be used in place of benzene.

III. *Fundamental Heterocyclic Compounds.*

14. Customary names of substances having terminations which are not in accordance with the chemical nature of the substances will undergo the following changes, which, however, may be modified to suit the requirements of individual languages.

(a) The termination *ol* will be changed to *ole.* Example : Pyrrole.

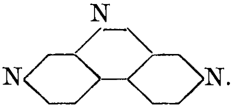
(b) The termination *ane* will be changed to *an.* Example : Pyran.

15. When a heterocyclic compound containing nitrogen but having a name not ending in *ine* gives basic compounds by progressive hydrogenation, such derivatives will be denoted by the successive terminations *ine, idine.* Examples : Pyrrole, pyrroline, pyrrolidine ; oxazole, oxazoline.

16. The termination *a* is to be used for the hetero-atoms in a ring, oxygen thus being denoted by *oxa*, sulphur by *thia*, nitrogen by *aza*, etc. The letter *a* may be omitted before a vowel. Examples : Thiadiazole, oxadiazole, thiazine, oxazine.

The names of heterocyclic compounds which are universally adopted will be retained, but the names of other heterocyclic compounds will be derived from those of the corresponding homocyclic compounds by adding the names of the hetero-atoms ending in *a.*

Example : 2 : 7 : 9-triazaphenanthrene,



IV. *Simple Functions.*

17. Substances of simple function are defined as those containing a function of one kind only, perhaps repeated several times in the molecule.

18. Where there is only one functional group, the fundamental chain will be selected so as to contain this group. Where there are several functional groups, the fundamental chain will be selected so as to contain the maximum number of these groups.

19. Halogenated derivatives will be designated by the name of the hydrocarbon from which they are derived, preceded by prefixes indicating the number and the nature of the halogens.

20. Alcohols and phenols will be given the names of the hydrocarbons from which they are derived, followed by the suffix *ol*. In accordance with rule 1, names universally adopted will be retained; phenol, cresol, naphthol, etc.

The nomenclature may be applied to heterocyclic hydroxy-compounds. Example: Quinolinol.

21. For the names of polyhydric alcohols and phenols, *di*, *tri*, *tetra*, etc., will be interposed between the name of the parent hydrocarbon and the suffix *ol*.

22. The name *mercaptan* as a suffix is abandoned; this function will be denoted by the suffix *thiol*.

23. Ether oxides are regarded as hydrocarbons in which one or more atoms of hydrogen are replaced by alkoxy-groups. For symmetrical ether oxides, however, the existing nomenclature will be retained. Examples: $CH_3{\cdot}O{\cdot}C_2H_5$ methoxyethane; $CH_3{\cdot}O{\cdot}CH_3$ methoxymethane or methyl ether.

24. Oxygen linked, in a chain of carbon atoms, to two of these atoms will be denoted by the prefix *epoxy* in all cases other than those in which a substance is named as a cyclic compound. Examples: ethylene oxide = epoxyethane; epichlorohydrin = 1 : 2-epoxy-3-chloropropane; tetramethylene oxide = 1 : 4-epoxybutane.

25. Sulphides, disulphides, sulphoxides and sulphones will be named in the same way as the ether oxides, *oxy* being replaced by *thio*, *dithio*, *sulphinyl*, and *sulphonyl* respectively. Examples: $CH_3{\cdot}SO_2{\cdot}C_2H_5$ methylsulphonylethane; $CH_3{\cdot}S{\cdot}C_3H_7$ methylthiopropane; $CH_3{\cdot}CH_2{\cdot}CH_2{\cdot}SO{\cdot}CH_2{\cdot}CH_2{\cdot}CH_2{\cdot}CH_3$ (1-propylsulphinyl)-butane.

26. Aldehydes are designated by the suffix *al* added to the names of the hydrocarbons from which they are derived; thioaldehydes by the suffix *thial*. Acetals will be named as 1 : 1-*dialkoxyalkanes*.

27. Ketones are to receive the termination *one*. Diketones,

triketones, thioketones will be designated by the suffix *dione, trione, thione.*

28. The name *keten* is retained.

29. For acids, the rules of the Geneva nomenclature are retained. However, where the use of this nomenclature results in cumbrous names, the carboxyl group is to be regarded as a substituent and the name of the acid will be made by adding the suffix *carbonic* or *carboxylic*, according to language, to the name of the hydrocarbon.

30. Acids in which an atom of sulphur replaces an atom of oxygen will be named according to the Geneva notation. Example: Ethane-thioic, -thiolic, -thionic, -thionthiolic. If the substituted carboxyl group is regarded as a substituent, the acids will be named *carbothioic* acids. The suffix *carbothiolic* is to be used if it is certain that the oxygen of the group OH is replaced by sulphur; the suffix *carbothionic* if oxygen of the group CO is so replaced; the suffix *carbodithioic* is to be used if the two oxygen atoms are replaced by sulphur.

31. The existing conventions will be retained for salts and esters.

32. Acid anhydrides will be named as anhydrides of the corresponding acids. For names formed according to the Geneva notation, amides, amidoximes, amidines, imides, and nitriles will be named in the same way as the acids, the terminations *amide, amidine, amidoxime, imide, nitrile* respectively being added to the name of the corresponding hydrocarbon. The acid halides will be named by combining chloride, etc., with the name of the radical. Examples: $C_3H_7{\cdot}COCl$ butanoyl chloride; $C_3H_7{\cdot}CO{\cdot}NH_2$ butanamide; etc.

When carboxyl is regarded as a substituent, the terminations *carbonamide, carbonamidine, carbonamidoxime, carbonimide, carbonitrile* are to be used. Examples: $C_3H_7{\cdot}COCl$ propanecarbonyl chloride; $C_3H_7{\cdot}CO{\cdot}NH_2$ propanecarbonamide.

33. The termination *ine* is reserved exclusively for nitrogenous bases. The existing nomenclature for monoamines is retained. The names of polyamines will be those of the hydrocarbons followed by the suffixes *di-*, *tri-amine.*

For aliphatic compounds containing quinquevalent nitrogen the termination *ine* will be changed to *onium.* For cyclic compounds containing quinquevalent nitrogen in the ring, the termination *ine* will be changed to *inium*; for those ending in *ole,* this will be changed to *olium.* Examples: Pyridine, pyridinium; imidazole, imidazolium.

34. The nomenclature of derivatives of phosphorus, arsenic, antimony and bismuth, being very complicated, will be considered later.

35. Compounds derived from hydroxylamine by replacement of

hydrogen of the hydroxyl will be regarded as alkoxy-derivatives; those in which an atom of hydrogen in the group NH_2 is replaced, as alkylhydroxylamines. Oximes will be named by adding the suffix *oxime* to the name of the corresponding aldehyde, ketone, or quinone. Examples: $C_2H_5{\cdot}O{\cdot}NH_2$ ethoxyamine; $C_2H_5{\cdot}NH{\cdot}OH$ ethylhydroxylamine.

36. The generic name *urea* is retained; it will be used as a suffix for alkyl and acyl derivatives and acids of urea. Examples: $C_4H_9{\cdot}NH{\cdot}CO{\cdot}NH_2$ butylurea; $C_3H_7{\cdot}CO{\cdot}NH{\cdot}CO{\cdot}NH_2$ butyrylurea.

The bivalent radical $NH{\cdot}CO{\cdot}NH$ is to be named *urylene.*

37. The generic name *guanidine* is retained.

38. The name *carbylamine* is retained.

39. *iso*Cyanic and *iso*thiocyanic esters (RNCO, RNCS) will be named iso*cyanates* and iso*thiocyanates.*

40. The name *cyanate* is reserved for true esters which on hydrolysis yield cyanic acid or its products of hydration. The name *thiocyanate* will be substituted for sulphocyanate (ide).

41. Nitro-derivatives: there is no change in the existing nomenclature.

42. Azo-compounds: the notation *azo, azoxy* is retained.

43. (a) Diazonium compounds $R{\cdot}N_2X$ will be named by adding the suffix *diazonium* to the name of the parent substance (hydrocarbon): benzenediazonium chloride.

(b) Compounds having the same empirical formula but containing tervalent nitrogen will be named by substituting *diazo* for *diazonium* (benzenediazohydroxide).

(c) Compounds of the type $R{\cdot}N_2{\cdot}OM$ will be named *diazoates.*

(d) Compounds in which the two atoms of nitrogen are linked to a single atom of carbon will be denoted by the prefix *diazo* (diazomethane, diazoacetic acid).

(e) The name *diazoamino* is retained; these substances, however, may be regarded as derivatives of triazene.

(f) Derivatives of the compounds

$$NH_2{\cdot}NH{\cdot}NH{\cdot}NH_2,\ NH{:}N{\cdot}NH{\cdot}NH_2,\ NH{:}N{\cdot}NH{\cdot}N{:}NH$$

will be named *tetrazanes, tetrazenes, pentazdienes,* etc.

44. Hydrazines will be designated by the name of the alcoholic radical from which they are derived, followed by the suffix *hydrazine.* In the cases where the amino-group of a carbonamide is replaced by the hydrazine-group the suffix *hydrazide* will be used.

Hydrazo-compounds are to be regarded as derivatives of hydrazine.

Examples: $CH_3{\cdot}NH{\cdot}NH_2$ methylhydrazine; $C_2H_5{\cdot}NH{\cdot}NH{\cdot}C_3H_7$ 1-ethyl-2-propylhydrazine; $C_3H_7{\cdot}CO{\cdot}NH{\cdot}NH_2$ butyrylhydrazine or propanecarbohydrazide.

45. Hydrazones and semicarbazones will be named in the same way as the oximes. The term *osazone* is retained.

46. The name *quinone* is retained.

47. Sulphonic and sulphinic acids will be designated by adding the suffix *sulphonic* or *sulphinic* to the name of the hydrocarbon.

The analogous acids of selenium and tellurium will be named *alkaneselenonic* and *alkaneseleninic* acids; *alkanetelluronic* and *alkanetellurinic.*

48. Organo-metallic compounds will be designated by the names of the organic radicals linked to the metal which they contain, followed by the name of the metal. Examples: Dimethylzinc, tetraethyllead, methylmagnesium chloride. However, if the metal is linked in a complex fashion, it may be regarded as a substituent. Example: $HgCl\cdot C_6H_4\cdot CO_2H$ chloromercuribenzoic acid.

49. The nomenclature of cyclic compounds having side chains will be considered later.

50. If it is necessary to avoid ambiguity, the names of complex radicals may be placed in parenthesis. Examples: $(CH_3)_2C_6H_3\cdot NH_2$ (dimethylphenyl)amine; $C_6H_5\cdot N(CH_3)_2$ phenyldimethylamine.

V. *Complex Functions.*

51. For compounds of complex function, that is, compounds which contain several radicals of different chemical character, the termination of the name will express only one kind of function (the principal function); the other functions will be designated by appropriate prefixes.

52. The following prefixes and suffixes will be used to designate the functions.

Function.	Prefix.	Suffix.
Acid and derivatives	Carboxy	carbonic (carboxylic), carbonyl, carbonamide, etc.; or oic, oyl, etc.
Alcohol	Hydroxy	ol
Aldehyde	Oxo, aldo (for O : aldehydic), or formyl (CHO)	al
Amine	Amino	amine
Quinquevalent nitrogen		onium, inium
Carbonitrile (nitrile)	Cyano	carbonitrile or nitrile
Ketone	Oxo or Keto	one
Azo-derivative	Azo	
Azoxy ,,	Azoxy	
Nitro- ,,	Nitro	
Nitroso- ,,	Nitroso	
Sulphinated derivative	Sulphino	sulphinic
Sulphonated ,,	Sulpho	sulphonic
Ether oxide	Alkoxy	
Halogenide	Halogeno	
Hydrazine	Hydrazino	hydrazine
Double linking		ene

Function.	Prefix.	Suffix.
Triple linking		yne
Mercaptan	Mercapto	thiol
Ethylene oxide, etc.	Epoxy	
Sulphones	Sulphonyl	
Sulphoxides	Sulphinyl	
Sulphides	Alkylthio	
Urea	Ureido	urea

53. The names of derivatives of the fundamental heterocyclic compounds will be formed according to the preceding rules.

VI. *Radicals.*

54. Univalent radicals derived from saturated aliphatic hydrocarbons by loss of one atom of hydrogen will be named by substitution of the termination *yl* for the termination *ane* of the hydrocarbon.

55. The names of univalent radicals derived from unsaturated hydrocarbons will end in *enyl, ynyl, dienyl,* etc., the positions of the double or triple linkings being indicated by numbers or letters, where this is necessary.

56. Bi- or ter-valent radicals derived from saturated hydrocarbons by loss of two or three atoms of hydrogen from the same atom of carbon will be named by substituting the termination *ylidene* or *ylidyne* for the termination *ane* of the hydrocarbon. For such radicals derived from unsaturated hydrocarbons, these terminations will be added to the name of the hydrocarbon. The names *iso*propylidene and methene are retained.

57. The names of bivalent radicals derived from aliphatic hydrocarbons by loss of one atom of hydrogen from each of the two terminal carbon atoms of the chain will be ethylene, trimethylene, tetramethylene, etc.

58. Radicals derived from acids by loss of the hydroxyl group will be named by changing the termination *carbonic* or *carboxylic* to *carbonyl,* or *oic* to *oyl* where the Geneva notation is used.

59. Univalent radicals derived from aromatic hydrocarbons by loss of an atom of hydrogen from the ring will in principle be named by changing the termination *ene* to *yl.* However, the radicals C_6H_5 and $C_6H_5{\cdot}CH_2$ will continue provisionally to be named *phenyl* and *benzyl* respectively. Moreover, certain abbreviations sanctioned by custom are authorised, such as *naphthyl* in place of *naphthalyl.*

60. Univalent radicals derived from heterocyclic compounds by loss of hydrogen from the ring will be named by changing the termination to *yl.* In cases where this would give rise to ambiguity, the final *e* will be simply changed to *yl.* Examples: Pyridine, pyridyl; indole, indolyl; pyrroline, pyrrolinyl; triazole, triazolyl; triazine, triazinyl.

61. Radicals formed by loss of an atom of hydrogen from a side chain of a cyclic compound will be regarded as substituted aliphatic radicals.

62. In general, special names will not be given to multivalent radicals derived from cyclic compounds by loss of several atoms of hydrogen from the ring. In such cases prefixes or suffixes will be used. Examples: Triaminobenzene or benzenetriamine; dihydroxypyrrole or pyrrolediol.

63. The order in which prefixes or radicals are to be named (alphabetical order or conventional) is optional.

VII. *Numbering.*

64. In aliphatic compounds the carbon atoms of the fundamental chain will be numbered from one end to the other, Arabic numerals being used. To avoid ambiguity the lowest numbers will be given (1) to the principal function, (2) to double linkings, (3) to triple linkings, (4) to atoms or radicals which are denoted by prefixes. The term " lowest number " signifies those which comprise it or the lowest individual numbers. For instance, 1 : 3 : 5- is less than 2 : 4 : 6-, 1 : 5 : 5- less than 2 : 2 : 6-, 1 : 2 : 5- less than 1 : 4 : 5-, 1 : 1 : 2 : 4- less than 1 : 3 : 4 : 4-.

65. Positions in side chains will be denoted by letters or numbers starting from the point of attachment. The letters or numbers together with the name of the chain will be given in parenthesis.

66. In cases of ambiguity in the numbering of atoms or radicals which are denoted by prefixes the order will be that which would be chosen for the prefixes before the name of the fundamental compound or of the side chain of which they are substituents.

67. The prefixes *di-*, *tri-*, *tetra-*, etc., will be used before simple expressions (for example, diethylbutanetriol) and the prefixes *bis*, *tris*, *tetrakis*, etc., before complex expressions. Examples: $CH_3{\cdot}NH{\cdot}[CH_2]_3{\cdot}NH{\cdot}CH_3$ bis(methylamino)propane; $(CH_3)_2N{\cdot}CH_2{\cdot}CH_2{\cdot}N(CH_3)_2$ bis(dimethylamino)ethane.

The prefix *bi* will only be used to denote the doubling of a radical or compound. For example, biphenyl.

68. A catalogue of cyclic systems and their numbering, based on the existing system and that of Mr. Patterson, is in course of preparation by the National Research Council of the United States of America and the American Chemical Society.

In order to avoid any confusion, the Committee recommends that a scheme of numbering be given at the foot of each memoir.