INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY
ORGANIC CHEMISTRY DIVISION
COMMISSION ON NOMENCLATURE OF ORGANIC CHEMISTRY

NOMENCLATURE OF ORGANIC CHEMISTRY

Sections A, B, C, D, E, F and H

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INTRODUCTION TO THE IUPAC REVISED AND COLLECTED RECOMMENDATIONS FOR THE NOMENCLATURE OF ORGANIC CHEMISTRY, 1978

The progress of the IUPAC Commission on the Nomenclature of Organic Chemistry during the period 1969 to 1977 has been reported in the Comptes Rendus of the Conferences (Recommended Rules) or in the Information Bulletin of the Union, Appendices on Provisional Nomenclature, Symbols, Units and Standards (Provisional Rules). While work for improving and completing nomenclature rules continues, we have now reached the point where it is possible and convenient to collect in a single volume a compendium of existing recommendations providing improved guidance to internationally agreed nomenclature.

The Sections included in this compendium are :

Section A. Hydrocarbons

Section B. Fundamental Heterocyclic Systems

Section C. Characteristic Groups containing Carbon, Hydrogen, Oxygen, Nitrogen, Halogen, Sulfur, Selenium and/or Tellurium

These Rules are the IUPAC Organic Nomenclature Rules Sections A, B and C, 1969, reprinted from the combined edition, Butterworths, London (1971), corrected for material errors.

Section D. Organic Compounds containing elements that are not exclusively Carbon, Hydrogen, Oxygen, Nitrogen, Halogen, Sulfur, Selenium and Tellurium.

These Rules are issued jointly by the Organic and Inorganic Nomenclature Commissions, and were published originally in IUPAC Information Bulletin, Appendix No.31, August 1973. Corrections for material errors and a few revisions have been introduced into the provisional text after evaluation of comments.

Section E. Stereochemistry

These Rules are IUPAC Recommendations 1974 and are reprinted from *Pure and Applied Chemistry*, Vol. 45, pp. 11-30 (Pergamon, 1976) with a few corrections for material errors.

Section F. General Principles for the Naming of Natural Products and Related Compounds

These Rules have not been finally approved, but their inclusion here seems appropriate (some minor errors have been corrected).

Section H. Isotopically Modified Compounds

These Rules, now approved, were originally published in the IUPAC Information Bulletin, Appendix No. 62, July 1977. Corrections for material errors have been introduced after evaluation of comments.

Although the titles of these Sections are to a large extent self-explanatory, it is thought useful here to make some comments on the arrangement of material. Glossaries of terms used are to be found in the Introduction to the 1969 Rules, p. xviii and in Section C, p. 81.

The attention of a reader having a nomenclature problem to solve is drawn first to Section C, which deals initially with general principles for the construction of a name. The operations described in this Section are usually to be applied to the names for hydrocarbons and heterocyclic systems provided by application of the Rules in Sections A and B.

Section D contains various types of material (see contents pp. ix-xii), some of which would be more appropriately included in earlier sections ; for example, much of Rules D-1 (Nomenclature Systems, p. 326), D-4 (Chains and Rings with Regular Patterns of Heteroatoms, p. 373), D-6 and D-7 (Organosilicon and Organoboron Compounds, pp. 409-458), and the Appendix Tables I, II and IV (pp. 459-471) falls into this category. We hope to reorganise the subject matter in a later edition.

INTRODUCTION TO 1969 EDITION OF SECTIONS A, B AND C

The first international proposals on the nomenclature of organic chemistry, made at Geneva in 1892, were revised and extended by the Definitive Report of the Commission for the Reform of Nomenclature in Organic Chemistry of the International Union of Chemistry (I.U.C.) which appeared after the meeting at Liége in 1930 (Liége Rules), and was supplemented by less extensive reports from the meetings at Lucerne in 1936 and at Rome in 1938. Although these proposals rendered great service, it was apparent at the meeting of the International Union of Pure and Applied Chemistry (I.U.P.A.C.) at London in 1947 that extension and revision of the nomenclature rules for organic chemistry were required.

Those who have served on the Commission on the Nomenclature of Organic Chemistry for varying periods from 1947 to 1969 are M. Betti*, R. S. Cahn, L. T. Capell, L. C. Cross, G. Dupont*, G. M. Dyson, C. S. Gibson*, H. Grünewald, G. Kersaint, S. P. Klesney, K. L. Loening, N. Lozac'h, R. Marquis*, A. D. Mitchell*, H. S. Nutting, A. M. Patterson*, V. Prelog, F. Richter*, J. Rigaudy, S. Veibel, P. E. Verkade, and E. Votoček*, and, as observers, K. A. Jensen (chairman, I.U.P.A.C. Commission on the Nomenclature of Inorganic Chemistry), W. Klyne (member of the IUPAC/IUB Commission for Biochemical Nomenclature).

The Commission's progress in the period 1947 to 1969, inclusive, has been reported in successive issues of the Comptes Rendus of the Conferences of the Union. Relevant parts of those reports are included, with a few revisions, in the rules which form the body of this publication.

Comments on these rules should be sent to the Secretary, S. P. Klesney, 3609 Boston, Midland, Michigan 48640, U.S.A. or to any other member of the Commission.

GENERAL PRINCIPLES

The Commission believes that differences in nomenclature frequently hinder the accurate and intelligible conveyance of information from one chemist to another, so tending to hamper understanding and progress. The Commission urges conformity with internationally agreed nomenclature even when this nomenclature may not seem the best possible from the point of view of the chemists of a particular nation or group.

The rules now presented are intended to be suitable for textbooks, journals and patents, for lexicons and similar compilations, and for indexes, even if not always wholly so for conversation or lectures. The rules will be issued in parts, as they become approved by the Union. They constitute recommendations for the naming of types of compounds and of individual compounds. They are not exhaustive, except in specified cases. Where, for various reasons, limitation to a single method of nomenclature appears undesirable or impossible, alternatives are given; but the Commission hopes that elimination of alternatives may become acceptable as the merits of one method become more generally recognized. The Commission hopes also that each nation will try to reduce the variations in nomenclature with regard to spelling, the position of numbers, punctuation, italicizing, abbreviations, elision of vowels, certain terminations, and so forth; the

* Deceased.

present rules are not to be held as making recommendations in these matters.

Owing to the very extensive nomenclature which has come into being since the last revision, the Commission has, in the main, confined its efforts to codifying sound practices which already existed, rather than to originating new nomenclature—the latter may form a later stage of the Commission's activities.

In so doing, the Commission had in mind the following main principles: (*a*) as few changes as possible should be made in existing nomenclature, though utility is more important than priority; (*b*) rules and names should be unequivocal and unique, but simple and concise; (*c*) records in journals, abstracts, compendia, and industry should be used to assess the relative extent of past use of various alternatives; (*d*) rules should be consistent with one another, yet aid expression in the particular field of chemistry involved and be capable of extension with the progress of science; (*e*) trivial names, and names having only a very small systematic component, cannot be eliminated when in very common use, but those of less value should be replaced by systematic (or at least more systematic) ones, and the creation of new trivial names should be discouraged by provision of extensible systematic nomenclature; (*f*) names should be adaptable to different languages. The Commission is aware that acceptance of its recommendations depends in large measure on the success which has attended its attempts to assess, for each particular case, the relative merits of these often conflicting claims.

GLOSSARY

The Commission considered it unnecessary to define chemical terms in common use. However, certain terms which have special meaning in nomenclature merit brief description; namely:

Parent compound: the principal chain or ring system from which a name is derived by substitution of hydrogen with other atoms or groups; e.g. methylcyclohexane has cyclohexane as its parent.

Systematic name: a name composed wholly of specially coined or selected syllables, with or without numerical prefixes; *e.g.*, pentane, oxazole.

Trivial name: a name no part of which is used in a systematic sense; *e.g.*, xanthophyll.

Semi-systematic name or semi-trivial name: a name of which only a part is used in a systematic sense; *e.g.*, methane (-ane), butene (-ene), calciferol (-ol). (Most names in organic chemistry belong to this class.)

Substitutive name: a name involving replacement of hydrogen by a group or by another element; *e.g.*, 1-methylnaphthalene, 1-pentanol.

Replacement name: an "a" name, where C, CH, or CH_2 is replaced by a hetero atom; *e.g.*, 2,7,9-triazaphenanthrene. Also, certain names

involving thio- (also seleno- or telluro-) to indicate replacement of oxygen by sulfur (or selenium or tellurium, respectively); *e.g.*, thiopyran.

Subtractive name: a name involving removal of specified atoms; *e.g.*, in the aliphatic series names ending in -ene or -yne. Also names involving anhydro-, dehydro-, deoxy-, *etc.*, or nor-.

Radicofunctional name: a name formed from the name of a radical and the name of a functional class; *e.g.*, acetyl chloride, ethyl alcohol.

Additive name: a name signifying addition between molecules and/or atoms; *e.g.*, styrene oxide.

Conjunctive name: a name formed by placing together the names of two molecules, it being understood that the two molecules are linked by loss of one hydrogen atom from each; *e.g.*, naphthaleneacetic acid.

Fusion name: a name for a cyclic system formed by use of a linking " o " between the names of two ring systems, denoting that the two systems are fused by two or more common atoms; *e.g.*, benzofuran.

Hantzsch–Widman name: a name for a heterocyclic system, derived from the original proposals of Hantzsch and Widman, and formed from a prefix or prefixes (to denote one or more hetero atoms) and a suffix -ole or -ine (to denote a five- or a six-membered ring, respectively); *e.g.*, triazole, thiazole.

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CONTENTS

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SECTION H

Isotopically Modified compounds