NOMENCLATURE OF ORGANIC CHEMISTRY

INTRODUCTION

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; the rules are written in accord with the conventions of *Chemical Abstracts* (except where specifically stated otherwise), but solely for uniformity from one rule to another.

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 name: that part of the name from which a particular name is derived by a prescribed variation; *e.g.*, ethane giving rise to ethanol. Names often have more than one parent; *e.g.*, (chloromethyl)cyclohexane has methylcyclohexane as parent, which in turn 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.

Bibliography

International Union of Pure and Applied Chemistry
Comptes rendus of the 9th Conference 1928, pp. 63–71
International Union of Chemistry
Comptes rendus of the 10th Conference 1930, pp. 57–64
Comptes rendus of the 12th Conference 1936, pp. 39–42
Comptes rendus of the 13th Conference 1938, pp. 36–37
Comptes rendus of the 14th Conference 1947, pp. 129–137
International Union of Pure and Applied Chemistry
Comptes rendus of the 15th Conference 1949, pp. 127–186
Comptes rendus of the 16th Conference 1951, pp. 100–104
Comptes rendus of the 18th Conference 1955, pp. 120–184

Patterson, A. M., Capell, L. T., and Walker, D. F. *The Ring Index*, 2nd ed., American Chemical Society, Washington, D.C., 1960

Hantzsch, A., and Weber, J. H., *Ber. Dtsch. Chem. Ges.* **20**, 3119 (1887)

Widman, O., *J. Prakt. Chem.*, [2], **38**, 185 (1888)

Baeyer, A., *Ber. Dtsch. Chem. Ges.* **33**, 3771 (1900)

CONTENTS

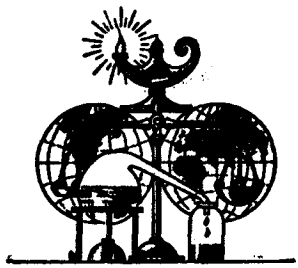
SECTION B

Fundamental Heterocyclic Systems

SECTION C

Characteristic Groups Containing Carbon, Hydrogen, Oxygen, Nitrogen, Halogen, Sulfur, Selenium, and/or Tellurium

Subsections



INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

NOMENCLATURE OF ORGANIC CHEMISTRY

DEFINITIVE RULES FOR
SECTION A. HYDROCARBONS
SECTION B. FUNDAMENTAL HETEROCYCLIC SYSTEMS

SECTION C. CHARACTERISTIC GROUPS CONTAINING
CARBON, HYDROGEN, OXYGEN, NITROGEN, HALOGEN,
SULFUR, SELENIUM, AND/OR TELLURIUM

Issued by the Commission on
the Nomenclature of Organic Chemistry

1969

LONDON
BUTTERWORTHS

PREFACE TO THE THIRD EDITION OF SECTIONS A AND B

This Third Edition of Sections A and B contains considerable changes from the Second Edition, but these have been confined, in the main, to correction of errors, to clarifications, in a few cases to expansion of existing Rules to cover special cases, and to provision of better or further examples.

However, major changes are the deletion of the Rules for order of complexity of side chains [Rule **A–2.3 (a)** and parts of Rules **A–2.4** and **A–2.5**] and of the Stelzner method of naming heterocyclic systems (Rule **B–4**) by replacement nomenclature ("a" nomenclature), because it is planned to abandon these procedures in Beilstein's *Handbuch der organischen Chemie* and they have been little used recently elsewhere.

Attention is also drawn to new Rules, in accord with principles of the other Rules, for naming heterocyclic ring assemblies (Rule **B–13**), for naming radicals derived from bridged compounds (**A–34.5** and **B–15**), from spiro compounds (**A–43** and **B–12**), from ring assemblies (**A–55** and **B–13**), and from compounds named by the von Baeyer system (**B–14**); there is also a new Rule, embodying *Ring Index* practice, for naming heterocyclic systems that contain one benzene ring and one hetero ring (**B–3.5**).

Other changes and additions that might have been made are reserved for inclusion in a major revision of nomenclature systems that is under consideration by the Commission.

The following constituted the Commission responsible for this (the Third) Edition: P. E. Verkade (Chairman), S. P. Klesney (Secretary), L. C. Cross, G. M. Dyson, K. L. Loening, N. Lozac'h, J. Rigaudy, S. Veibel, with, as Associate Members, R. S. Cahn, H. Grünewald, and, as Observers, K. A. Jensen (Chairman, I.U.P.A.C. Commission on the Nomenclature of Inorganic Chemistry) and W. Klyne (Member of the I.U.P.A.C./I.U.B. Commission for Biochemical Nomenclature).

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

A. HYDROCARBONS

ACYCLIC HYDROCARBONS

Rule A-1. Saturated Unbranched-chain Compounds and Univalent Radicals

1.1—The first four saturated unbranched acyclic hydrocarbons are called methane, ethane, propane and butane. Names of the higher members of this series consist of a numerical term, followed by "-ane" with elision of terminal "a" from the numerical term. Examples of these names are shown in the table below. The generic name of saturated acyclic hydrocarbons (branched or unbranched) is " alkane ".

Examples of names:

(n = total number of carbon atoms)

n		n		n	
1	Methane	15	Pentadecane	29	Nonacosane
2	Ethane	16	Hexadecane	30	Triacontane
3	Propane	17	Heptadecane	31	Hentriacontane
4	Butane	18	Octadecane	32	Dotriacontane
5	Pentane	19	Nonadecane	33	Tritriacontane
6	Hexane	20	Eicosane	40	Tetracontane
7	Heptane	21	Heneicosane	50	Pentacontane
8	Octane	22	Docosane	60	Hexacontane
9	Nonane	23	Tricosane	70	Heptacontane
10	Decane	24	Tetracosane	80	Octacontane
11	Undecane	25	Pentacosane	90	Nonacontane
12	Dodecane	26	Hexacosane	100	Hectane
13	Tridecane	27	Heptacosane	132	Dotriacontahectane
14	Tetradecane	28	Octacosane		

1.2—Univalent radicals derived from saturated unbranched acyclic hydrocarbons by removal of hydrogen from a terminal carbon atom are named by replacing the ending " -ane " of the name of the hydrocarbon by " -yl ". The carbon atom with the free valence is numbered as 1. As a class, these radicals are called normal, or unbranched chain, alkyls.

Examples:

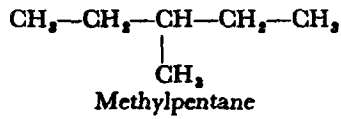
Pentyl $\overset{5}{CH_3}—\overset{4}{CH_2}—\overset{3}{CH_2}—\overset{2}{CH_2}—\overset{1}{CH_2}—$

Undecyl $\overset{11}{CH_3}—\overset{10\text{-}2}{[CH_2]_9}—\overset{1}{CH_2}—$

Rule A-2. Saturated Branched-chain Compounds and Univalent Radicals

2.1—A saturated branched acyclic hydrocarbon is named by prefixing the designations of the side chains to the name of the longest chain present in the formula.

Example:



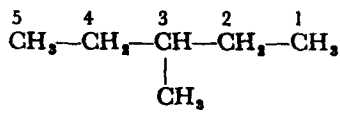
Methylpentane

The following names are retained for unsubstituted hydrocarbons only:

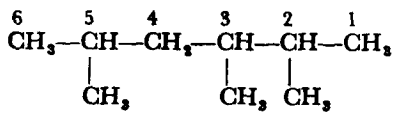
Isobutane	$(CH_3)_2CH—CH_3$
Isopentane	$(CH_3)_2CH—CH_2—CH_3$
Neopentane	$(CH_3)_4C$
Isohexane	$(CH_3)_2CH—CH_2—CH_2—CH_3$

2.2—The longest chain is numbered from one end to the other by arabic numerals, the direction being so chosen as to give the lowest numbers possible to the side chains. When series of locants containing the same number of terms are compared term by term, that series is " lowest " which contains the lowest number on the occasion of the first difference. This principle is applied irrespective of the nature of the substituents.

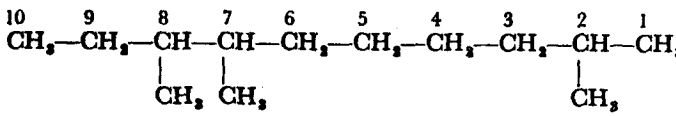
Examples:



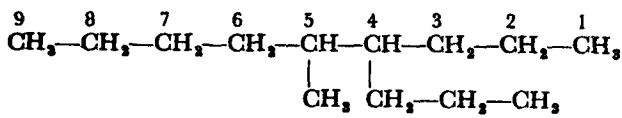
3-Methylpentane



2,3,5-Trimethylhexane (not 2,4,5-Trimethylhexane)



2,7,8-Trimethyldecane (not 3,4,9-Trimethyldecane)



5-Methyl-4-propylnonane
(not 5-Methyl-6-propylnonane because 4,5 is lower than 5,6)

2.25—Univalent branched radicals derived from alkanes are named by prefixing the designation of the side chains to the name of the unbranched alkyl radical possessing the longest possible chain starting from the carbon atom with the free valence, the said atom being numbered as 1.

Examples:

1-Methylpentyl $\overset{5}{CH_3}\overset{4}{CH_2}\overset{3}{CH_2}\overset{2}{CH_2}\overset{1}{CH}(CH_3)—$

2-Methylpentyl $CH_3CH_2CH_2CH(CH_3)CH_2—$

5-Methylhexyl $(CH_3)_2CHCH_2CH_2CH_2CH_2—$

The following names are retained for the unsubstituted radicals only:

Isopropyl $(CH_3)_2CH—$

Isobutyl $(CH_3)_2CH—CH_2—$

sec-Butyl $CH_3—CH_2—\underset{\displaystyle CH_3}{\overset{\displaystyle |}{CH}}—$

tert-Butyl $(CH_3)_3C—$

Isopentyl $(CH_3)_2CH—CH_2—CH_2—$

Neopentyl $(CH_3)_3C—CH_2—$

tert-Pentyl $CH_3—CH_2—\underset{\displaystyle CH_3}{\overset{\displaystyle CH_3}{\overset{\displaystyle |}{\underset{\displaystyle |}{C}}}}—$

Isohexyl $(CH_3)_2CH—CH_2—CH_2—CH_2—$

2.3—If two or more side chains of different nature are present, they are cited in alphabetical order.*

The alphabetical order is decided as follows:

(*i*) The names of simple radicals are first alphabetized and the multiplying prefixes are then inserted.

Example:

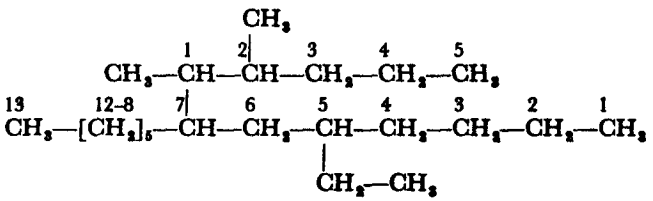
$$\overset{7}{CH_3}—\overset{6}{CH_2}—\overset{5}{CH_2}—\overset{4}{CH}(\overset{\displaystyle 3}{\overset{\displaystyle CH_3—CH_2}{\overset{\displaystyle |}{\underset{\displaystyle |}{C}}}}\overset{\displaystyle CH_3}{\overset{\displaystyle |}{\underset{\displaystyle CH_3}{|}}})—\overset{2}{CH_2}—\overset{1}{CH_3}$$

ethyl is cited before methyl, thus **4-Ethyl-3,3-dimethylheptane**

*Use of an order of complexity given as alternative in the First and Second Editions is abandoned.

(*ii*) The name of a complex radical is considered to begin with the first letter of its complete name.

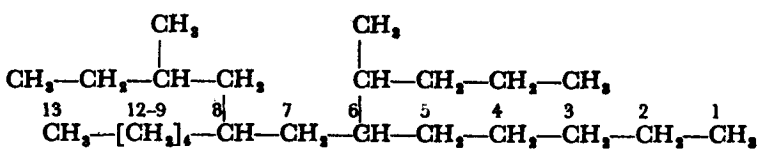
Example:



dimethylpentyl (as a complete single substituent) is alphabetized under "d", thus 7-(1,2-Dimethylpentyl)-5-ethyltridecane

(*iii*) In cases where names of complex radicals are composed of identical words, priority for citation is given to that radical which contains the lowest locant at the first cited point of difference in the radical.

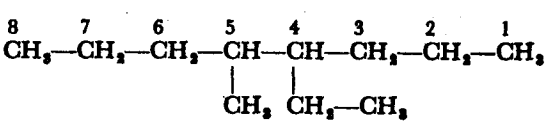
Example:



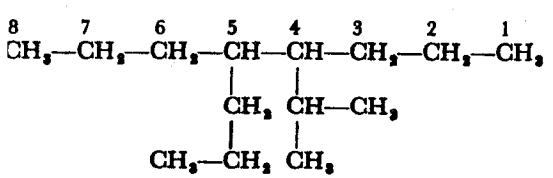
6-(1-Methylbutyl)-8-(2-methylbutyl)tridecane

2.4—If two or more side chains are in equivalent positions, the one to be assigned the lower number is that cited first in the name.

Examples:



4-Ethyl-5-methyloctane



4-Isopropyl-5-propyloctane