



Brief Guide to the Nomenclature of Organic Chemistry

K.-H. Hellwich (Germany), R. M. Hartshorn (New Zealand), A. Yerin (Russia), T. Damhus (Denmark), A. T. Hutton (South Africa). E-mail: organic.nomenclature@iupac.org Sponsoring body: IUPAC Division of Chemical Nomenclature and Structure Representation.

1 INTRODUCTION

The universal adoption of an agreed nomenclature is a key tool for efficient communication in the chemical sciences, in industry and for regulations associated with import/export or health and safety. The International Union of Pure and Applied Chemistry (IUPAC) provides recommendations on many aspects of nomenclature.¹ The basics of organic nomenclature are summarized here, and there are companion documents on the nomenclature of inorganic² and polymer³ chemistry, with hyperlinks to original documents. An overall summary of chemical nomenclature can be found in *Principles of Chemical Nomenclature*.⁴ Comprehensive detail can be found in *Nomenclature of Organic Chemistry*, colloquially known as the Blue Book,⁵ and in the related publications for inorganic compounds (the Red Book),⁶ and polymers (the Purple Book).⁷ It should be noted that many compounds may have non-systematic or semi-systematic names and IUPAC rules also allow for more than one systematic name in many cases. Some traditional names (e.g. styrene, urea) are also used within systematic nomenclature. The new edition of the Blue Book⁸ incorporates a hierarchical set of criteria for choosing the single name which is to be preferred for regulatory purposes, the Preferred IUPAC Name, or PIN.

2 SUBSTITUTIVE NOMENCLATURE

Substitutive nomenclature is the main method for naming organic-chemical compounds. It is used mainly for compounds of carbon and elements of Groups 13–17. For naming purposes, a chemical compound is treated as a combination of a parent compound (Section 5) and characteristic (functional) groups, one of which is designated the principal characteristic group (Section 4). A systematic name is based on the name of the most senior parent compound (Section 6) in which the substitution of hydrogen atoms is represented by a suffix for the principal characteristic group(s), prefixes representing less senior characteristic groups and other substituent groups, and locants that specify their locations. Names created according to substitutive nomenclature may also include fragments named in accordance with other nomenclature types or operations. For example, addition and subtraction operations (Section 5.4) are performed mainly to define the hydrogenation state, while a replacement operation defines a replacement of (in most cases) carbon atoms with heteroatoms.

2.1 Components of systematic substitutive names

The most common components of a substitutive chemical name are illustrated with reference to the chemical structure shown in Table 1, along with its systematic name and the components of the name. Locants indicate the position of substituents or other structural features. They are generally placed before the part of the name that indicates the corresponding structural feature. Three kinds of enclosing mark are used, in the nesting order [] ({ }), when it is necessary to indicate which parts of a name belong together.

Table 1: Components of the substitutive name
(4*S*,5*E*)-4,6-dichlorohept-5-en-2-one for



hept(a)	parent (heptane)	one	suffix for principal characteristic group
one(b)	unsaturation ending	chloro	substituent prefix
di	multiplicative prefix	S, E	stereodescriptors
4, 5, 6	locants		enclosing marks

Multiplicative prefixes (Table 2) are used when more than one fragment of a particular kind is present in a structure. Which kind of multiplicative prefix is used depends on the complexity of the corresponding fragment – e.g. trichloro, but tris(chloromethyl).

Table 2: Multiplicative prefixes for simple/complicated entities

No.	Simple	Complicated	No.	Simple	Complicated
2	di	bis	8	octa	octakis
3	tri	tris	9	nona	nonakis
4	tetra	tetrakis	10	deca	decakis
5	penta	pentakis	11	undeca	undecakis
6	hexa	hexakis	12	dodeca	dodecakis
7	hepta	heptakis	20	icosa	icosakis

3 CREATION OF SYSTEMATIC NAMES

The formation of a systematic name requires several steps, to be taken (when they are applicable) in the following order:

- Determine the principal characteristic group to be cited as the suffix (see Section 4).
- Determine the senior parent amongst those structural components attached to a principal characteristic group (see Sections 5 and 6).
- Name the parent hydride and specify any unsaturation (Section 5).
- Combine the name of the parent hydride with the suffix for the principal characteristic group (Section 4).
- Identify the substituents and arrange the corresponding prefixes in alphabetical order.
- Insert multiplicative prefixes, without changing the already established order, and insert locants.
- Determine chirality centres and other stereogenic units, such as double bonds, and add stereodescriptors.

4 CHARACTERISTIC GROUPS – Suffixes and prefixes

The presence of a characteristic (or functional) group is denoted by a prefix or suffix attached to the parent name. The names of common characteristic groups are given in Table 3, in order of decreasing seniority. The most senior one, the principal characteristic group, is cited as the suffix, while all other groups are cited as prefixes. Note that, for nomenclature purposes,

Table 3: Seniority order for characteristic groups

Class	Formula*	Suffix	Prefix
Carboxylates	–COO (–COO) [–]	carboxylate oate	carboxylate
Carboxylic acids	–COOH (–COOH)	carboxylic acid oic acid	carboxy
Esters	–COOR (–COOR)	(R) –carboxylate** (R) –oate**	(R)oxycarbonyl
Acid halides	–COX (–COX)	carboxyl halide oyl halide	halocarbonyl
Amides	–CONH ₂ (–CONH ₂)	carbamamide amide	carbamoyl
Nitriles	–C≡N (–C≡N)	carbonitrile nitrile	cyano
Aldehydes	–CHO (–CHO)	carbaldehyde al	formyl oxal
Ketones	–O–	one	oxo
Alcohols	–OH	ol	hydroxy
Thiols	–SH	thiol	sulfanyl***
Amines	–NH ₂	amine	amino
Imines	–NH–	imine	imino

* Here –(C) indicates that the carbon atom is implied by the parent name.

** Here (R) means that the group R is expressed as a separate prefixed word.

*** Note: ‘mesocapto’ is no longer acceptable (but is still used by CAS).



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* Freely available at: <http://www.dogriya.com/view/jpac>

(a) <https://www.iupac.org.uk/about/iupac/>

(b) R. M. Hartshorn et al., *Brief Guide to the Nomenclature of Inorganic Chemistry*, *Pure Appl. Chem.*, 879–106, 1039–1049 (2015).

(c) R. C. Haines et al., *A Brief Guide to Polymer Nomenclature*, *Pure Appl. Chem.*, 841–90, 2167–2169 (2015).

(d) *Principles of Chemical Nomenclature – A Guide to IUPAC Recommendations*, 2nd Edition, G. J. Leigh (Ed.), RSC Publishing, Cambridge, U.K., ISBN 978-1-84973-007-5.

(e) *Nomenclature of Organic Chemistry – IUPAC Recommendations and Preferred Names 2013*, H. A. Ison, M. H. Purnell (Eds.), Royal Society of Chemistry, Cambridge, U.K., ISBN 978-0-95454-182-8, <https://www.iupac.org.uk/about/iupac/>

(f) *Nomenclature of Organic Chemistry – IUPAC Recommendations 2005*, N. G. Connolly, T. Damhus, R. M. Hartshorn, A. T. Hutton (Eds.), RSC Publishing, Cambridge, U.K., ISBN 0-85404-438-8.

(g) *Compendium of Polymer Terminology and Nomenclature – IUPAC Recommendations 2006*, R. G. Jones, J. Kabovici, R. Nappo, E. S. Wilson, M. Hoss, T. Kotayama, W. V. Meeks (Eds.), RSC Publishing, Cambridge, U.K., ISBN 978-0-85404-495-7.

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