1 Directions for Use of the Book

The present Book is a practical nomenclature manual for all those confronted with the task of formulating or understanding even the most complicated names of organic, organometallic, and coordination compounds in a straightforward manner, i.e., advanced chemistry and pharmacy students; chemists, pharmacologists, and biochemists; scientists at all levels in both academia and industries; documentalists, editors, and software developers. The Book does not recommend any new nomenclature rules but provides help to navigate through the nomenclature jungle by means of a comprehensive and clear representation of existing rules and recommendations. Also the historical development of chemical nomenclature, or the reasons for a specific name or its etymological significance are not treated. The interested reader should consult the literature[1)].

In the last years, several companies have developed computer software which allows the generation of systematic names from drawn structure diagrams and vice versa, see *§ A.1.12*[2)3)4)5)6)]. Computer software is generally suitable for the naming of simpler organic compounds, but knowledge of chemical nomenclature is indispensable for checking of the names produced. Name interpretation with software is problematic since it requires the input of a correct name.

§ A.1.12

The *International Union of Pure and Applied Chemistry* (IUPAC) has rendered outstanding service to the chemical community by its publications of nomenclature recommendations, in particular of the so-called '*Blue Book 1979*', i.e., *Nomenclature of Organic Chemistry 1979*[7)], and the *Guide to IUPAC Nomenclature of Organic Compounds, Recommendations 1993*[8)]. These have considerably contributed to the creation of internationally accepted nomenclatures for organic compounds. A re-edition of these recommendations has been published early in 2014: *Nomenclature of Organic Chemistry, IUPAC Recommendations and Preferred Names 2013*[9)]. Most of the IUPAC recommendations published after 1979 have been incorporated into the '*Blue Book 2013*'[9)]. An important change in these 2013 recommendations is the concept of a 'Preferred IUPAC Name' (PIN); however, any name other than a PIN is still acceptable as a 'general IUPAC name' as long as it is unambigous and follows the principals of IUPAC recommendations. The present Book provides numerous updates of IUPAC names, and corresponding references to the '*Blue Book 2013*' appear in the main part of the Book in the margin of the pages as 'IUPAC P'. More recent IUPAC recommendations and revisions of older recommendations are regularly published by IUPAC in *Pure and Applied Chemistry* and are accessible via the Internet (*§ A.1.12*). A general introduction to the IUPAC recommendations has appeared in 1998[10)]. The revised IUPAC recommendations for naming inorganic compounds have been published in 2005 as a new '*Red Book*'[11)]. Brief guides to the nomenclature of organic and inorganic chemistry have appeared in 2020 and 2015[12)].

IUPAC P-....

§ A.1.12

The most frequently used database for the retrieval of chemical information is set up by the American Chemical Society's *Chemical Abstracts Service* (CA). For this database (CAS Registry^{SM}), CA selects a single preferred name for a given compound, the so-called index name that is listed in its former 'Chemical Substance Index' and accessible by CA's SciFinder® interface or STN® network. In SciFinder®, in addition to the index name with the corresponding formula, CA lists other names and even abbreviations used in the primary literature for a given compound. For the index names, CA has developed a nomenclature that is based on IUPAC recommendations. Contrary to widespread opinion, the index names of CA are in general compatible with IUPAC recommendations. The rules for the selection of the index names are summarized in CA's *Index Guide*, *Appendix IV*[13)], which has appeared in general every two years and which refers to the index names of the corresponding period of time.

1) P.E. Verkade, 'A History of the Nomenclature of Organic Chemistry', D. Reidel Publishing Company, Dordrecht – Boston – Lancaster, 1985.

2) Advanced Chemistry Development Inc., Toronto, Canada, 'ACD/Name' (see *§ A.1.12*).

3) ChemInnovation Software Inc., San Diego, CA, USA, 'Nomenclator' and 'NamExpert', in 'Chemistry 4-D Draw' (see *§ A.1.12*).

4) PerkinElmer, Inc., Waltham, MA, USA, in 'ChemDraw Professional' (see *§ A.1.12*).

5) iChemLabs, Chesterfield, VA USA, in 'ChemDoodle' (see *§ A.1.12*).

6) ChemAxon, Budapest, Hungary, in 'Marvin Sketch' (see *§ A.1.12*).

7) International Union of Pure and Applied Chemistry, Organic Chemistry Division, 'Nomenclature of Organic Chemistry, Sections A–F and H', Pergamon Press, Oxford – New York – Toronto – Sydney – Paris – Frankfurt, 1979; IUPAC recommendations A–F and H.

8) International Union of Pure and Applied Chemistry, Organic Chemistry Division, 'A Guide to IUPAC Nomenclature of Organic Compounds, Recommendations 1993', Blackwell Scientific Publications, Oxford – London – Edinburgh – Boston – Melbourne – Paris – Berlin – Vienna, 1993 (errata in *Pure Appl. Chem.* **1999**, *71*, 1328); IUPAC recommendations R.

9) International Union of Pure and Applied Chemistry, H.A. Favre, W.H. Powell, 'Nomenclature of Organic Chemistry, Recommendations and Preferred Names 2013', RSC Publishing, Cambridge, UK, 2014; accessible, incl. errata, via <https://iupac.org>; IUPAC recommendations P.

10) G.J. Leigh, H.A. Favre, W.V. Metanomski, 'Principals of Chemical Nomenclature, a Guide to IUPAC Recommendations', Blackwell Science Ltd., Oxford – London – Edinburgh – Malden – Victoria – Paris – Berlin – Tokyo, 1998.

11) International Union of Pure and Applied Chemistry, 'Nomenclature of Inorganic Chemistry, IUPAC Recommendations 2005', RSC Publishing, Cambridge, UK, 2005; accessible via <https://iupac.org>

12) International Union of Pure and Applied Chemistry, 'Brief Guide to the Nomenclature of Organic Chemistry', *Pure Appl. Chem.* **2020**, *92*, 527; International Union of Pure and Applied Chemistry, 'Brief Guide to the Nomenclature of Inorganic Chemistry', *Pure Appl. Chem.* **2015**, *87*, 1039; both accessible via <http://www.qmul.ac.uk/sbcs/iupac>.

13) American Chemical Society, 'Chemical Abstracts, Index Guide, Appendix IV', Chemical Abstracts Service, Columbus, Ohio, last print edition 2004.

Changes in CA's nomenclature guidelines have been infrequent and always clearly reported. A major update of CA's nomenclature has occurred in 2007, at the time when the present Book has been published for the first time. These 2007 guidelines, *Naming and Indexing of Chemical Substances for Chemical Abstracts 2007*[14], are available as pdf file from CA's website. References to these latest CA guidelines appear in the main part of this Book in the margin of the pages as 'CA ¶'. In reality, the collection of these rules is not a nomenclature manual but a collection of (restricting) nomenclature guidelines for the user of the CA indexes or databases, allowing the user to proceed from the structure of a compound to the place of its registration in the 'Chemical Substance Index' or CAS Registry[SM] and vice versa.

CA ¶ ...

1

The present *Book is based on the nomenclature guidelines used by CA* for the choice of index names but also contains most IUPAC-accepted trivial names and references to IUPAC's 2013 recommendations. Deviations from the CA guidelines for names in this Book concern the *noninversion of the name components* (see (g) in *§ 3.1*) and the *position of locants in names* (see *§ 3.4*) to improve clarity.

§ 3.1 (g)
§ 3.4

This Book is structured in such a way that in most instances one can give an appropriate name to a structure or derive the structure from the name by means of the letter rules (a), (b), (c), etc., of the *Instructions* and the information given under *Notice*, i.e., by means of the main part of the Book. In the case of more complicated names, one can reach these objectives by using the supplementary material given in footnotes and appendixes or by studying the many examples. In addition to the references to the CA guidelines and the IUPAC recommendations, references to other paragraphs (§) and Tables of the Book also appear in the margin.

Instructions

(a)

The art of perfect name construction or name interpretation resides in the skill of correctly analyzing and classifying the structure of a compound or of a name, respectively, before name construction or name interpretation is attempted. Sometimes it is helpful to *start with a simpler structure of the same kind* rather than naming the complicated structure right away.

- For the assignment of a name to a structure, *the structure is dissected into constitutional structure components* that are named separately. These name components are then assembled into the whole name according to specific guidelines.
- For the derivation of the structure from a given name, *the name is dissected into the individual name components* to which constitutional structure components are assigned. *Start the analysis at the end of the name!*

(b)

The names of most organic compounds consist, in general, of three components:

prefixes + parent name + suffix[15]
or
prefixes + parent-substituent name + functional-parent name[15]

The names of organometallic and coordination compounds consist similarly of two components:

ligand names + central-atom name[15]

On the whole, the necessary information for name construction and name interpretation can be found in three parts of the Book:

- *§ 3* contains the **general instructions** for name construction and interpretation, in particular the rules for the choice of the **senior compound class** (→ prefixes, suffix or functional-parent name; central-atom and ligand names; *§ 3.1*) and for the choice of the **molecular-skeleton parent** (→ parent name; *§ 3.3*) or of the **parent substituent** (→ parent-substituent name; *§ 5.8*)**.** An important support is *Tab. 3.2* which includes a seniority list of compound classes and the most frequently encountered suffixes, functional-parent names, and prefixes. Further prefixes can be found in *Tab. 3.1*. — § 3; § 3.1; § 3.3; § 5.8, Tab. 3.2; Tab. 3.1
- *§ 4* contains a collection of molecular-skeleton parents, with instructions for the formation of corresponding parent names and parent-substituent names. Parent-substituent names are also summarized in *§ 5*. — § 4; § 5
- *§ 6* contains the detailed description of the individual compound classes with their suffixes or functional-parent names and corresponding prefixes, and with central-atom names and ligand names. — § 6

The appendixes *(§ A.1–A.9)* supply further useful information. — § A.1–A.9

(c)

The instructions of the Book must be applied systematically in the given order. Do not skip intermediate steps!

Notice

- In every subsection (e.g., *§ 3.1*, *§ 3.2*, etc.; *§ A.1.1*, *§ A.1.2*, etc.), the numbering of the formulas or formula names and of footnotes begins with **1** and **1)**, respectively, except for the short *§ 5*. — § 3.1, 3.2; § A.1.1, A.1.2; § 5
- In the context of hierarchy rules, the **sign** > means senior, i.e., the structure or name component in front of > is senior.
- In a name, **boldface printing** serves only to highlight the corresponding name component, and the **sign** ~ within a name at the end of a line means the absence of a hyphen at this place in the name; all other hyphens are part of the name. An **arrow** → means: 'the name becomes ...', see, e.g., *§ 5*, except if present inside a name. — § 5

14) American Chemical Society, 'Naming and Indexing of Chemical Substances for Chemical Abstracts 2007', Chemical Abstracts Service, Columbus, Ohio, last edition 2007; see <https://www.cas.org> (site search: 'Naming' leads to 'Naming and Indexing of Chemical Substances for Chemical Abstracts'; CA guidelines ¶.

15) The basic terms of chemical nomenclature used in this Book, e.g., prefix, suffix, etc., are explained in *§ 2.1. Some terms differ from those used by CA and/or IUPAC;* corresponding cross references are given in *§ 2.1* which must be consulted in case of doubt.

- The annotation IUPAC generally refers to IUPAC recommendations on which CA rules are based or which differ from them.
- In structural formulas, the following abbreviations are occasionally used: **Me– for CH_3–**, **Et– for CH_3CH_2–**, and **Ph– for C_6H_5–**.
- The general name components alkyl, aryl, and acyl mean:

  alkyl = monovalent group, formed by formal removal of an H atom from the C atom of an aliphatic (also heteroatom-containing) molecular-skeleton parent, see *§ 4.2–4.5*, *4.7*, *4.9*, and *4.10*, e.g., Me–.

§ 4.2–4.5, 4.7, 4.9, 4.10

  aryl = monovalent group, formed by formal removal of an H atom from the C atom of an aromatic (also heteroatom-containing) molecular-skeleton parent, see *§ 4.5*, *4.6,* and *4.8–4.10*), e.g., Ph–.

§ 4.5, 4.6, 4.8–4.10

  acyl = mono- or polyvalent group, formed by formal removal of one (or several) OH group(s) and/or chalcogen analog(s) from an acid, see *§ 6.7–6.12*, e.g., MeC(=O)–, MeC(=S)–, $MeS(=O)_2$–, PH(=O)(OH)–, PH(=O)<.

§ 6.7–6.12

- The *structural formulae of five- and seven-membered ring components in fused polycycles are not always represented as regular polygons* because of the naming procedure (see *§ 4.6*). A wavy line ξ in a sketched formula of a substituent indicates one or more terminal free valences.

§ 4.6

2 FUNDAMENTALS

2.1 Nomenclature Terms and Definitions Used in the Book[1)]

§3.2.4 **Additive name** **(1)** Name in which atoms added to the *molecular-skeleton parent* are expressed as a *prefix* such as additional H atoms, i.e., no atoms are substituted. E.g.

'1,2-dihydronaphthalene' ($C_{10}H_{10}$).

(2) Name in which the name components of component parts of a structure are juxtaposed like these component parts, without expressing the loss of atoms such as H atoms from these component parts, i.e., no atoms are substituted. E.g.,

'pyridine 1-oxide' ($C_5H_5N{=}O$),
'triamminetrichlorocobalt' ($[CoCl_3(NH_3)_3]$),
'methyllithium' (MeLi).

IUPAC[2)] attributes a more extensive meaning to this term.

Affix An affix (≠ *prefix*, *infix*, or *suffix*) modifies the name part which it precedes; the affix is not detachable from this name part (see also *multiplying affix*). E.g.,

'thio' in 'thiosulfuric acid' (e.g., $HS{-}S(=O)_2{-}OH$),
'peroxy' in 'peroxysulfamic acid' ($H_2N{-}S(=O)_2{-}OOH$).

IUPAC[2)] uses the term affix as a collective term for prefixes and suffixes. CA[3)] uses the term affix for infixes.

'a' Name See *replacement name.*

'a' Prefix See *heteroatom syllable.*

'a' Syllable See *heteroatom syllable.*

§4.6.3 **Attached component** Non*senior* ring component of a polycyclic *molecular-skeleton parent* with a *fusion name*.

Base component Term formerly used for *parent component.*

'Blue Book 2013' [2)] IUPAC's 2013 nomenclature recommendations of organic chemistry. 'Blue Book 1979' refers to the corresponding 1979 recommendations (obsolete).

§A.7 **Bonding number** The bonding number *n* is the sum of the valence bonds of a molecular-skeleton atom and is indicated in a name by the symbol λ*ⁿ* (*lambda convention*).

Cahn–Ingold–Prelog (CIP)

§A.6.2 **System** System developed by R.S. Cahn, C.K. Ingold, and V. Prelog and used for the specification of the configuration of a stereogenic center, a stereogenic axis (including chirality plane), or a stereogenic double bond, which allows the indication of a stereodescriptor '*R*'/'*S*', '*P*'/'*M*', '*E*'/'*Z*', etc., in the name of a stereoisomer.

CA Name[3)] Name assigned according to the Chemical Abstracts (CA) nomenclature guidelines for CA indexes and their database, see '*Index Guide*' and *CAS Registry*℠.

CAS Registry℠ CAS Registry℠ is the database of CA which contains more than 175 million unique organic and inorganic chemical substances (January 2021), i.e., a collection of disclosed chemical-substance information covering substances identified from the scientific literature since the early 1800s up to the present. This information is displayable and searchable by means of CA's SciFinder® and STN® network.

§6.34 **Central atom** Atom in a central position of a coordination compound which is bonded to other atoms or groups of atoms, i.e., to *ligands*. E.g.,

Co in $[Co(NH_3)_6]^{3+}$ ('hexaamminecobalt(3+)'),
Co in $[CoF_3(NH_3)_3]$ ('triamminetrifluorocobalt'),
Co in $[CoCl_4]^{2-}$ ('tetrachlorocobaltate(2–)').

For nomenclature purposes, the metal atom of an organometallic compound is treated here like a central atom. E.g.,

Li in MeLi ('methyllithium').

§3.1 **Characteristic** (or functional) **group** *Substituent* that is not bound by a C–C bond to a *molecular-skeleton parent* or a *parent substituent.* See also *isolated group*. E.g.,

–OH, =O, $-NH_2$, $-P(=O)(OH)_2$, etc.

Substituents formally derived from a carboxylic acid substituent, ions, and radicals (species with unpaired electrons) are also considered to be characteristic groups. E.g.,

–COOH, –COOR, –CN, –CH(=O), –C(=O)X with X = Hal,
NH_2, NHR, etc., and corresponding chalcogen analogs.

In hydrocarbon chains and their heteroanalogs as well as in carbo- and heterocycles, *unsaturations and heteroatoms are,* for nomenclature purposes, *not considered to be characteristic groups*.

Nonfunctional compounds without characteristic groups are polyazanes, hydroxylamines, polyphosphines, phosphine oxide, phosphines, etc., silanes, etc., ▶▶

1) *Some nomenclature terms used in this Book are different from those used by CA and/or IUPAC.* Corresponding cross references are given in this section, which must be consulted in case of doubt. For instance, the term prefix is restricted here to substituent prefixes. Indeed, the use of 'a' prefix (IUPAC) or replacement prefix (IUPAC and CA) for what is termed heteroatom syllable in this Book is confusing and can lead to incorrect replacement names in which the heteroatom syllables are arranged in alphabetical order (see *§ 3.5*) rather than according to their seniority (see, e.g., *§ 4.3.2*).

2) International Union of Pure and Applied Chemistry, H.A. Favre, W.H. Powell, 'Nomenclature of Organic Chemistry, Recommendations and Preferred Names 2013', RSC Publishing, Cambridge, UK, 2014; accessible, incl. errata, via <https://iupac.org>. The corresponding IUPAC recommendations are indicated in the margin as 'IUPAC P'.

3) American Chemical Society, 'Naming and Indexing of Chemical Substances for Chemical Abstracts 2007', Chemical Abstracts Service, Columbus, Ohio, last edition 2007; <https://www.cas.org> (site search: 'Naming'). CA Guidelines are indicated in the margin as 'CA ¶'.

boranes, polyoxides, peroxides, polysulfones, polysulfoxides, polysulfides, etc. E.g.,
$H_2N–NH–NH_2$, $NH_2–OH$, $H_2P–PH_2$, $PH_3=O$, PH_3, SiH_4, BH_3,
R–O–O–O–R′, R–O–O–R′, $R–S(=O)_2–S(=O)_2–R′$,
R–S(=O)–S(=O)–R′, R–S–S–R′.

§6.34 **Charge number** Arabic numeral followed by the sign of the charge (+ or –) which is placed directly after the name of an ion to indicate the size of the ionic charge. E.g.,
'hexaamminecobalt(3+)' ($[Co(NH_3)_6]^{3+}$),
'tetrafluoroborate(1–)' ($[BF_4]^-$),
'iron(3+) [hexakis(cyano-κ*C*)ferrate(3–)] (1:1)' ($Fe[Fe(CN)_6]$).

§A.6.4 **Chirality symbol** Part of the *stereodescriptor* of a coordination compound (see also *polyhedral symbol, configuration number,* and *ligand segment*) which describes the absolute configuration of the stereogenic *central atom* and allows the distinction of enantiomers by the descriptors '*R*'/'*S*', 'Δ'/'Λ', or '*C*'/'*A*'. E.g.,
final '*C*' in '(*OC*-6-65-*C*)-'.

CIP System See *Cahn–Ingold–Prelog system*.

e.g., §6.22 **Class name** Name of the principal group in a *functional-class name* consisting of a *parent-substituent name* and an *ending* (i.e., class name). E.g.,
'hydroperoxide' (–O–OH) in 'ethyl hydroperoxide' (Et–O–OH).

e.g., §6.15 **Class term** Part of a *functional-parent name*. E.g.
'acid' in 'phosphonic acid' ($PH(=O)(OH)_2$),
'chloride' in 'carbonic dichloride' (Cl–C(=O)–Cl).

§5.8 **Composite prefix** Name of a composite *substituent*, formed by juxtaposing simple *prefixes* or by means of substitutive nomenclature. E.g.
'(pentyloxy)-' ($MeCH_2CH_2CH_2CH_2O–$),
'(chlorocarbonyl)-' (ClC(=O)–),
'(1-methylethyl)-' ($Me_2CH–$),
'(methylamino)-' (MeNH–).
IUPAC[2] and CA[3] use the terms compound prefix or complex prefix.

§6.34 **Configuration number** (configuration index) Part of the *stereodescriptor* of a coordination compound (see also *polyhedral symbol*, *chirality symbol*, and *ligand segment*) which consists of *priority numbers* and describes the positions of the individual coordinating atoms at the corners of the coordination polyhedron. It allows the distinction of diastereoisomers. E.g,
the configuration number '2' in '(*SP*-4-2)-' indicates that in a square-planar coordination compound '(*SP*-4)', the coordinating atom of priority number ② is in *trans* position to the coordinating atom of priority number ①.

§3.2.2 **Conjunctive name** Name for a structure in which an arbitrary ring component is connected by a single bond to a functionalized hydrocarbon-chain component (carrying a group expressed as a *suffix*) implying the loss of an H atom from each component. The ring component and the hydrocarbon-chain component together form the *molecular-skeleton parent*. E.g.,
'cyclohexaneacetic acid' ($C_6H_{11}–CH_2COOH$),
'pyridine-2-propanol' ($C_5H_4N–CH_2CH_2CH_2OH$).

§6.34 **Coordination number** (coordination valence) Number of formal σ bonds (also by means of lone pairs of electrons) that are possible in a coordination compound between the central atom and the ligands (i.e., number of coordinating ligand atoms). E.g.,
Co^{III} has the coordination number 6 in $[Co(NH_3)_6]^{3+}$.

§A.7 **Delta** (δ) **convention** Convention for the description of a molecular-skeleton atom in a cyclic *molecular-skeleton parent* at which cumulated (contiguous) double bonds converge, by means of the descriptor δ^c where *c* is the number of double bonds at this molecular-skeleton atom.

§2.2.2 **Elision** Omission of a vowel of *heteoatom syllables, multiplying affixes, infixes,* or *attached-component* names when followed by vowels.

§2.2.1 **Enclosing marks** They are used to set off name components.

§3.1 **Ending** *Suffix, functional-parent name,* or *class name* for the designation of the *principal group*. E.g.,
'-ol' in 'ethanol' (Et–OH),
'-phosphonic acid' in '*P*-ethylphosphonic acid' ($Et–P(=O)(OH)_2$),
'hydroperoxide' in 'ethyl hydroperoxide' (Et–O–OH).
IUPAC[2] recommends this term, among others, for the last syllable of a *molecular-skeleton parent name* (see *final syllable*).

§6.34 **Eta** (η) **descriptor** (hapto symbol, η symbol) Part of a *ligand name* which describes the coordination sites of the *ligand* of a coordination compound. E.g.,
'(η^3-prop-2-en-1-yl)' ($[\mathbf{CH_2CHCH_2}]^-$).

§6.34 **Ewens–Bassett number** See *charge number*.

Final syllable Last syllable of a *molecular-skeleton parent name*. E.g.,
'-ene' in 'but-2-ene' (MeCH=CHMe),
'-ole' in 'oxazole' (C_3H_3NO),
'-epine' in '1,4-thiazepine' (C_5H_5NS).

§3.2.6 **Functional-class name**[4] Name in which the *principal group* is expressed as a *class name* (i.e., *ending*), and the 'parent structure' is treated as a *substituting group* (formerly called *radical*), i.e., as a *parent substituent*. E.g.,
'ethyl hydroperoxide' (Et–O–OH).
IUPAC[2] attributes a more extensive meaning to this term.

Functional group See *characteristic group*.

Functional modifier See *modification*.

Functional parent See *parent structure*.

§3.3, Tab. 3.2 **Functional-parent name**[4] **(1)** Name of a *functional parent*. E.g.,
'carbonic acid' (HO–C(=O)–OH),
'phosphonic acid' ($PH(=O)(OH)_2$).

§3.2.1 **(2)** Name of the principal group in a *substitutive name* composed of one or several *parent-substituent names* and an *ending* (i.e., functional-parent name). E.g.,
'-phosphonic acid' ($–P(=O)(OH)_2$) in '*P*-ethylphosphonic acid' ($Et–P(=O)(OH)_2$).

4) A similar procedure is used when giving a *functional-class name* (see functional-class nomenclature, *§3.2.6*) or a *functional-parent name* (see substitutive nomenclature, *§3.2.1*): the name of the parent substituent precedes (in alphabetical order if two are needed) the name of the principal group (e.g., 'hydroperoxide' or '-phosphonic acid', resp.).