Systematic Nomenclature of Organic, Organometallic and Coordination Chemistry

Chemical-Abstracts Guidelines with IUPAC Recommendations and Many Trivial Names

Ursula Bünzli-Trepp

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Logos Verlag Berlin GmbH
Georg-Knorr-Str. 4, Geb. 10
D-12681 Berlin
Tel.: +49 (0)30 / 42 85 10 90
Fax: +49 (0)30 / 42 85 10 92
https://www.logos-verlag.com

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℠), 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℠ 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.

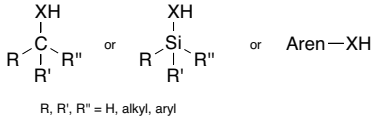
§ 4.6

CA ¶ 175, 229, 291
IUPAC P-63.1

6.21 Alcohols and Phenols (Class 10)

Definition

An alcohol or phenol **1** has a substituent –XH (X = O, S, Se, Te) *at a C or Si atom* of a molecular-skeleton parent. In the following, the term alcohol is employed as a general expression for all chalcogeno replacement analogs **1** (X = O, S, Se, Te).



1 an alcohol or phenol (X = O)
a thiol (X = S)
a selenol (X = Se)
a tellurol (X = Te)

According to the degree of substitution, an alcohol is designated generally as:

primary alcohol	RCH_2–OH	(R ≠ H)
secondary alcohol	RCH(R′)–OH	(R, R′ ≠ H)
tertiary alcohol	RC(R′)(R″)–OH	(R, R′, R″ ≠ H)

Notice

- If possible, conjunctive nomenclature according to *§ 3.2.2* must be employed, see **11**, **27**, **28**, **34**, **40**, **73**, **75**, **76**, and **78** – **80**. (§ 3.2.2)
- Hemiacetals RC(R′)(XR″)XH (X = O, S, Se, Te; R″ ≠ H) are designated as alcohols, see **41** and **42**.
- Alcoholates R–X^- are described in (c) of *§ 6.4.2.2* and ethers R–X–R′ (X = O, S, Se, Te) in *§ 6.30* and *6.31*. (§ 6.4.2.2 (c), § 6.30, 6.31)

Instructions are given for:

(a) alcohols and phenols with the substituent –XH (X = O, S, Se, Te) at a C or Si atom: suffixes and substituent prefixes (exception: 'phenol'; trivial names 'ethylene glycol', 'glycerol', 'pentaerythritol', 'pinac~ol', 'cresol', 'carvacrol', 'thymol', 'pyrocatechol', 'resorcinol', 'hydroquinone', 'picric acid', 'naphthol', 'anthrol', 'phenanthrol');
(b) nontraditional alcohols with the substituent HX– (X = O, S, Se, Te) at a heteroatom (≠ Si): substituent prefixes;
(c) nontraditional esters with the substituent acyl–X– (X = O, S, Se, Te) at a heteroatom (≠ Si): ester names;
(d) ether substituents R–X– (X = O, S, Se, Te; R = alkyl, aryl, silyl): substituent prefixes.

Instructions

(a) *Alcohols and phenols*

The name of an alcohol or phenol **R–XH** (X = O, S, Se, Te; R = alkyl, aryl, silyl), i.e., with *–XH at a C or Si atom*, consists of:

parent name of the molecular-skeleton parent **R–H**, by *§ 4.2–4.10* (§ 4.2–4.10)
+
suffix

'-**ol**'	(–OH)
'-**thiol**'	(–SH)
'-**selenol**'	(–SeH)
'-**tellurol**'	(–TeH)

If necessary, multiplying affixes are employed, e.g., 'ethane-1,2-diol' ($HOCH_2CH_2OH$).

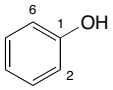
Aromatic alcohols **arene–OH** and chalcogen analogs are also designated as alcohols, e.g., **16**–**26**, *except* for 'phenol' (**2**) and its derivatives. Hemiacetals **RC(R′)(OR″)OH** and chalcogen analogs are substituted alcohols, see **41** and **42**.

The prefix for an alcohol substituent **HX–** (H atom not substitutable) at a molecular-skeleton parent is:

prefix

'**hydroxy**-'	(HO–)
'**mercapto**-'	(HS–)
'**selenyl**-'	(HSe–)
'**telluryl**-'	(HTe–)

Exception (a)



2 '**phenol**'
H at C substitutable, but not by Ph (see ring assemblies, *§ 4.10*); e.g., Ph–C_6H_4–OH is '[1,1′-biphenyl]-4-ol'

IUPAC recommends for PINs of alcohols and phenols names similar to those of CA (P-63.1.2 and P-63.1.5); the trivial name '**phenol**' (**2**) is a PIN (P-63.1.1.1). For alcohols with –XH = –OH also functional-class names (*§ 3.2.6*) are accepted as non-PINs (P-63.1.2; see **3**–**11** (for trivial substituent prefixes, see *§ 4.2* and *4.4*–*4.6*)).

The following trivial names are still accepted as non-PINs: '**ethylene glycol**' (**12**), '**glycerol**' (**13**), '**pentaerythritol**' (**14**), '**pinacol**' (**15**), '**cresol**' (see **16**), '**carvacrol**' (**17**), '**thymol**' (**18**), '**pyrocatechol**' (**19**), '**resorcinol**' (**20**), '**hydroquinone**' (**21**), '**picric acid**' (**22**), '**naphthol**' (see **23**), and '**anthrol**' (see **24**), but *not* '**phenanthrol**' (see **25**) (P-63.1.1.2).

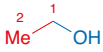
Since 1978, the **carbinol** nomenclature is obsolete ('Blue Book 1978', C-201.1; see **28**). The affixes 'thio-', 'seleno-', and 'telluro-' in connection with trivial names are no longer employed, and instead of the formerly recommended substituent prefixes 'mercapto-' (HS-) and '(hydroseleno)-' (HSe–), the preferred prefixes '**sulfanyl**-' (HS–), '**selanyl**-' (HSe–), and '**tellanyl**-' (HTe–) must be used; the CA prefixes are not recommended (P-63.1.5).

Names of **α-amino alcohols** can be derived from the names of the corresponding α-aminocarboxylic acids (P-103.2.8), e.g.,
'L-alaninol' (L-$MeCH(NH_2)CH_2OH$),
'L-glutaminol' (L-$H_2NC(O)CH_2CH_2CH(NH_2)CH_2OH$).

Examples (a)

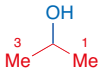
3 'methanol'

IUPAC: also '**methyl alcohol**' (P-63.1.2); substitutable



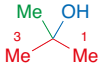
4 'ethanol'

IUPAC: also '**ethyl alcohol**' (P-63.1.2); substitutable



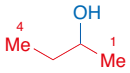
5 'propan-2-ol'

- IUPAC: also '**isopropyl alcohol**' (P-63.1.2); not substitutable
- *not* 'isopropanol'



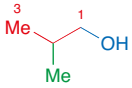
6 '2-methylpropan-2-ol'

- IUPAC: also '***tert*-butyl alcohol**' (P-63.1.2); not substitutable
- *not* '*tert*-butanol'



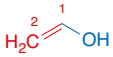
7 'butan-2-ol'

- IUPAC: no longer '***sec*-butyl alcohol**' (P-29.6.3)
- *not* '*sec*-butanol'



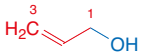
8 '2-methylpropan-1-ol'

- IUPAC: no longer '**isobutyl alcohol**' (P-29.6.3)
- *not* 'isobutanol'



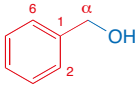
9 'ethenol'

IUPAC: also '**vinyl alcohol**' (P-63.1.2); substitutable



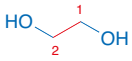
10 'prop-2-en-1-ol'

IUPAC: also '**allyl alcohol**' (P-63.1.2); substitutable



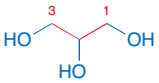
11 'benzenemethanol'

- conjunctive name
- IUPAC: 'phenylmethanol' (PIN; P-63.1.2); also '**benzyl alcohol**', substitutable only at the ring



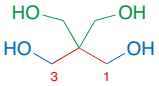
12 'ethane-1,2-diol'

IUPAC: also '**ethylene glycol**' (P-63.1.1.2); not substitutable



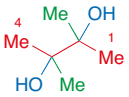
13 'propane-1,2,3-triol'

IUPAC: also '**glycerol**' (P-63.1.1.2); not substitutable



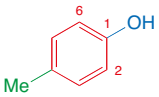
14 '2,2-bis(hydroxymethyl)propane-1,3-diol'

IUPAC: also '**pentaerythritol**' (P-63.1.1.2); not substitutable



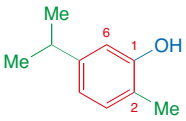
15 '2,3-dimethylbutane-2,3-diol'

IUPAC: also '**pinacol**' (P-63.1.1.2); not substitutable; 'pinacol' was also used as a general name for vicinal diols



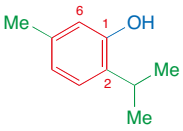
16 '4-methylphenol'

IUPAC: also '***p*-cresol**' (P-63.1.1.2); similarly for '*o*-' and '*m*-cresol'; not substitutable



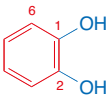
17 '2-methyl-5-(1-methylethyl)phenol'

IUPAC: also '**carvacrol**' (P-63.1.1.2); not substitutable



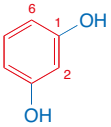
18 '5-methyl-2-(1-methylethyl)phenol'

IUPAC: also '**thymol**' (P-63.1.1.2); not substitutable



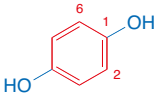
19 'benzene-1,2-diol'

- IUPAC: also '**pyrocatechol**' (P-63.1.1.2); not substitutable; the trivial name '**guaiacol**' (= '2-methoxyphenol') for *o*-MeO–C_6H_4–OH is no longer accepted
- trivially also '**catechol**'



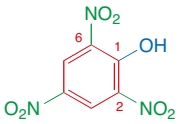
20 'benzene-1,3-diol'

IUPAC: also '**resorcinol**' (P-63.1.1.2); not substitutable



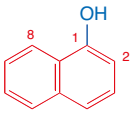
21 'benzene-1,4-diol'

- IUPAC: also '**hydroquinone**' (P-63.1.1.2); not substitutable
- formerly also 'hydroquinol'



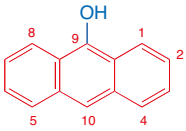
22 '2,4,6-trinitrophenol'

IUPAC: also '**picric acid**' (P-63.1.1.2); not substitutable



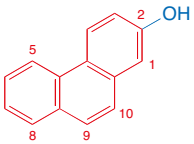
23 'naphthalen-1-ol'

IUPAC: also '**1-naphthol**' (P-63.1.1.2); not substitutable



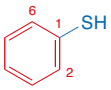
24 'anthracen-9-ol'

IUPAC: also '**9-anthrol**' (P-63.1.1.2); not substitutable



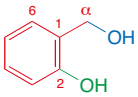
25 'phenanthren-2-ol'

IUPAC: no longer '**2-phenanthrol**' (P-63.1.1.2)



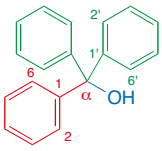
26 'benzenethiol'

formerly '**thiophenol**'



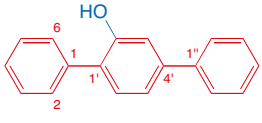
27 '2-hydroxybenzenemethanol'

- conjunctive name
- choice of the molecular-skeleton parent by (e) of *§ 3.3*
- IUPAC: '2-(hydroxymethyl)phenol' (PIN; P-44.1.2.2, i.e., ring > chain)
- trivially '**salicyl alcohol**'



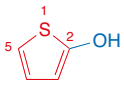
28 'α,α-diphenylbenzenemethanol'

- conjunctive name
- IUPAC: 'triphenylmethanol' (PIN; P-13.5.2); also '**trityl alcohol**' (P-63.1.2 and P-29.6.2.2), not substitutable
- *not* '**triphenylcarbinol**'



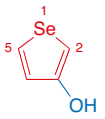
29 '[1,1′:4′,1″-terphenyl]-2′-ol'

not '2,5-diphenylphenol'



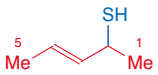
30 'thiophene-2-ol'

CA: 'thiophene-2-ol'; no elision of 'e' to avoid confusion with the formerly used trivial name 'thiophenol' (PhSH; **26**)

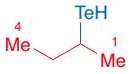


31 'selenophene-3-ol'

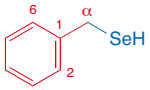
CA: 'selenophene-3-ol'; no elision of 'e' to avoid confusion with the formerly used trivial name 'selenophenol' (PhSeH); analogously for 'tellurophene-3-ol'



32 'pent-3-ene-2-thiol'

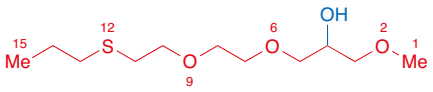


33 'butane-2-tellurol'

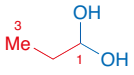


34 'benzenemethaneselenol'

- conjunctive name
- IUPAC: 'phenylmethaneselenol' (PIN; P-15.6.1.1)

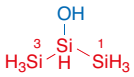


35 '2,6,9-trioxa-12-thiapentadecan-4-ol'



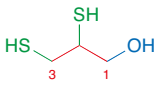
36 'propane-1,1-diol'

an **aldehyde hydrate**



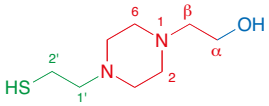
37 'trisilan-2-ol'

38 '1-methylsilacyclobutan-1-ol'



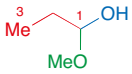
39 '2,3-dimercaptopropan-1-ol'

IUPAC: '2,3-bis(sulfanyl)propan-1-ol' (PIN; P-63.1.5)



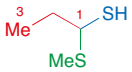
40 '4-(2-mercaptoethyl)piperazine-1-ethanol'

- conjunctive name
- IUPAC: '2-[4-(2-sulfanylethyl)piperazin-1-yl]ethan-1-ol' (PIN; P-63.1.5)



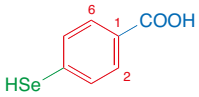
41 '1-methoxypropan-1-ol'

- a **hemiacetal**
- IUPAC: also 'propanal methyl hemiacetal' (P-66.6.5.2)



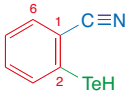
42 '1-(methylthio)propane-1-thiol'

- a **dithiohemiacetal**
- IUPAC: '1-(methylsulfanyl)propane-1-thiol' (PIN; P-63.1.5); also 'propanal methyl dithiohemiacetal' (P-66.6.5.4)



43 '4-selenylbenzoic acid'

IUPAC: '4-selanylbenzoic acid' (PIN; P-63.1.5)



44 '2-tellurylbenzonitrile'

IUPAC: '2-tellanylbenzonitrile (PIN; P-63.1.5)

(b) *Nontraditional alcohols*

A substituent **HX–** (X = O, S, Se, Te) attached at a heteroatom different from an Si atom of a heterochain or heterocycle **Y–H** is treated as a **nontraditional alcohol**. Its name consists of:

prefix

'**hydroxy**-'	(HO–)
'**mercapto**-'	(HS–)
'**selenyl**-'	(HSe–)
'**telluryl**-'	(HTe–)

+

parent name of the heterochain or heterocycle **Y–H**, by *§ 4.3* or *4.5–4.10*

§ 4.3, 4.5–4.10

The senior compound class (not necessarily an alcohol!) is then determined by possibly present other substituents, see **52** or **94**. Note that HX– groups which are part of an acid function are not concerned (see acids of the *Classes 5c*, *5e–g*, *5j*, and *5k* in *Tab. 3.2*, e.g., 'methanesulfonic acid' (Me–S(=O)$_2$–OH), 'sulfuric acid' (HO–S(=O)$_2$–OH), 'phosphonic acid' (HP(=O)(OH)$_2$), 'phosphinous acid' (H$_2$P–OH), 'borinic acid' (H$_2$B–OH).

Tab. 3.2

§ 6.25–6.29

Nontraditional alcohols are also described in *§ 6.25–6.29* dealing with the N, P, As, Sb, Bi, B, Ge, Sn, and Pb compounds of the *Classes 14–20* (see *Tab. 3.2*).

Tab. 3.2

CA ¶ 193

Exceptions (b)

45 '**hydroxylamine**'

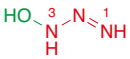
least senior compound of *Class 14* (*§ 6.25*); **45** is a special molecular-skeleton parent, i.e., a nontraditional alcohol; an *O*-alkyl or *O*-aryl derivative R–O–NH$_2$ is denoted by a prefix (with locant '*O*'); an *O*-acyl derivative acyl–O–NH$_2$ is an azanyl ester (see (b$_0$) and (c) of *§ 6.14*); an *N*-alkylidene derivative R=N–OH is an oxime (see *§ 6.19* and *6.20*); an *N*-alkyl or *N*-aryl derivative R–NH–OH is an amine (see *§ 6.23*); an *N*-acyl derivative acyl–NH–OH is an amide (see *§ 6.16*); see *§ 6.25* for some derivatives of **45**

46 '**thiohydroxylamine**'

- least senior compound of *Class 14* (*§ 6.25*); **46** is a special molecular-skeleton parent; see **45** for derivatives; however, an *S*-alkyl or *S*-aryl derivative R–S–NH$_2$ is a sulfenamide (see *§ 6.16*)
- correspondingly for the Se and Te analogs: '**selenohydroxylamine**' (H$_2$N–SeH) and '**tellurohydroxylamine**' (H$_2$N–TeH)

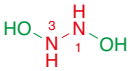
IUPAC recommends for PINs of nontraditional alcohols (= 'heterols') to use the suffixes '-ol', etc., instead of the prefixes (P-63.1.3 and P-63.1.5). For PINs of hydroxylamines, see P-68.3.1.1.1 and errata in
https://www.qmul.ac.uk/sbcs/iupac/bibliog/BBerrors.html

Examples (b)



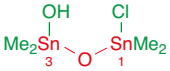
47 '3-hydroxytriaz-1-ene'

IUPAC: 'triaz-2-en-1-ol' (PIN; P-63.1.3)



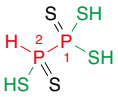
48 '1,2-dihydroxyhydrazine'

IUPAC: 'hydrazine-1,2-diol' (PIN; P-63.1.3)



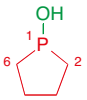
49 '1-chloro-3-hydroxy-1,1,3,3-tetramethyl~distannoxane'

IUPAC: '3-chloro-1,1,3,3-tetramethyldistannoxan-1-ol' (PIN; P-63.1.3)



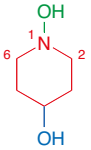
50 '1,1,2-trimercaptodiphosphine 1,2-disulfide'

- additive name (=S at P^{III}); cf. (d) of *§ 6.20*
- IUPAC: '1,1,2-tris(sulfanyl)-1λ^5,2λ^5-diphosphane-1,2-dithione' (PIN; P-68.3.2.2 and P-68.3.2.3.1)



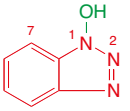
51 '1-hydroxyphospholane'

IUPAC: 'phospholan-1-ol' (PIN; P-63.1.3)



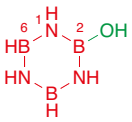
52 '1-hydroxypiperidin-4-ol

- *not* 'piperidine-1,4-diol'
- IUPAC: 'piperidine-1,4-diol' (PIN; P-63.1.3)



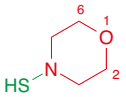
53 '1-hydroxy-1*H*-benzotriazole'

- indicated H atom by (a) and (d) of *§ A.5*
- abbreviation: '**HOBt**'
- IUPAC: '1*H*-1,2,3-benzotriazol-1-ol' (PIN; P-63.1.3)



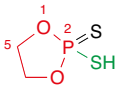
54 '2-hydroxyborazine'

IUPAC: '1,3,5,2,4,6-triazatriborinan-2-ol' (PIN; P-68.1.1.3.2 and P-63.1.3)



55 '4-mercaptomorpholine'

IUPAC: 'morpholin-4-thiol' (PIN; P-63.1.3)



56 '2-mercapto-1,3,2-dioxaphospholane 2-sulfide'

- additive name (=S at P^{III}); cf. (d) of *§ 6.20*
- IUPAC: '2-sulfanyl-1,3,2λ^5-dioxaphospholane-2-thione' (PIN; P-68.3.2.2 and P-68.3.2.3.1)

(c) *Nontraditional esters*

§ 6.14 (b_0) (c)

A substituent **acyl–X–** (X = O, S, Se, Te) attached at a heteroatom different from an Si atom of a heterochain or heterocycle **Y–H** is treated as a **nontraditional ester** **acyl–X–Y** according to (b_0) and (c) of *§ 6.14*, and *no longer* similarly to a nontraditional alcohol (see (b)). Notice that, as an exception, an **acyl–X–N=CRR′** is named as an **oxime** of an aldehyde or ketone, e.g., 'propan-2-one *O*-acetyloxime' (MeC(=O)–O–N=CMe$_2$; cf. (b) of *§ 6.19* and (e) of *§ 6.20*).

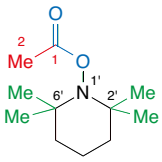
§ 6.19 (b), § 6.20 (e)

§ 6.25–6.29

Nontraditional esters are also described in *§ 6.25–6.29* dealing with the N, P, As, Sb, Bi, B, Ge, Sn, and Pb compounds of the *Classes 14–20* (see *Tab. 3.2*).

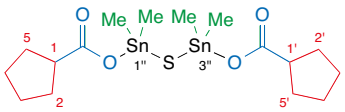
Tab. 3.2

Examples (c)



57 'acetic acid 2,2,6,6-tetramethylpiperidin-1-yl ester'/'2,2,6,6-tetramethylpiperidin-1-yl acetate'

ester; see ester definition in (b_0) and (c) of *§ 6.14*, i.e., ester of a common acid and a nontraditional alcohol



'**58** 'cyclopentanecarboxylic acid 1,1′-(1,1,3,3-tetramethyldistannathiane-1,3-diyl) ester'/'1,1′-(1,1,3,3-tetramethyldistannathiane-1,3-diyl) bis[cyclopentanecarboxylate]'

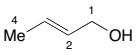
ester; see ester definition in (b_0) and (c) of *§ 6.14*, i.e., ester of an exotic acid and a nontraditional alcohol

(d) *Ether-substituent prefixes*

§ 5.8 § 6.30, 6.31

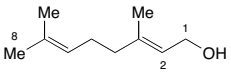
The prefix of a substituent **R–X–** (X = O, S, Se, Te; R = alkyl, aryl, silyl) is a composite prefix and built according to *§ 5.8* (see *§ 6.30* and *6.31*). Note that the trivial names '**methoxy**-' (MeO–), '**ethoxy**-' (EtO–), '**propoxy**-' (MeCH$_2$CH$_2$O–), '**butoxy**-' (MeCH$_2$CH$_2$CH$_2$O–), and '**phenoxy**-' (PhO–) are used.

Additional Examples



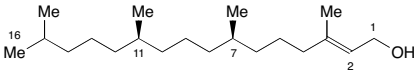
59 'but-2-en-1-ol'

- by (a)
- formerly trivially '**crotyl alcohol**'



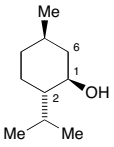
60 '(2*E*)-3,7-dimethylocta-2,6-dien-1-ol'

- by (a)
- '(2*E*)' by *§ A.6.3*
- trivially '**geraniol**'



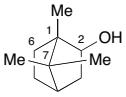
61 '(2*E*,7*R*,11*R*)-3,7,11,15-tetramethylhexadec-2-en-1-ol'

- by (a)
- '(2*E*,7*R*,11*R*)' by *§ A.6.3*
- trivially '**phytol**'



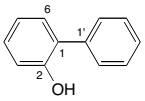
62 '(1*R*,2*S*,5*R*)-5-methyl-2-(1-methylethyl)cyclohexanol'

- by (a)
- '(1*R*,2*S*,5*R*)' by *§ A.6.3*
- trivially '**(1*R*)-menthol**'



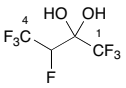
63 '1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol'

- by (a)
- trivially '**borneol**'



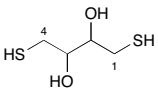
64 '[1,1′-biphenyl]-2-ol'

- by (a)
- not '2-phenylphenol'



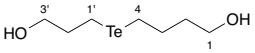
65 '1,1,1,3,4,4,4-heptafluorobutane-2,2-diol'

- by (a)
- a **ketone hydrate**



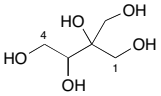
66 '1,4-dimercaptobutane-2,3-diol'

by (a)



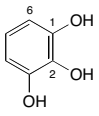
67 '4-[(3-hydroxypropyl)telluro]butan-1-ol'

- by (a)
- C_4 chain > C_3 chain

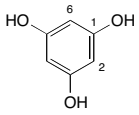


68 '2-(hydroxymethyl)butane-1,2,3,4-tetrol'

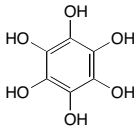
by (a)



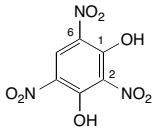
69 'benzene-1,2,3-triol'
- by (a)
- formerly trivially '**pyrogallol**'



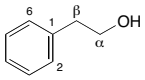
70 'benzene-1,3,5-triol'
- by (a)
- formerly trivially 'phloroglucinol' or '**phloroglucin**'



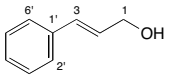
71 'benzene-1,2,3,4,5,6-hexol'
by (a)



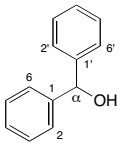
72 '2,4,6-trinitrobenzene-1,3-diol'
- by (a)
- formerly trivially '**styphnic acid**'



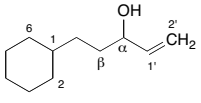
73 'benzeneethanol'
- by (a)
- conjunctive name
- IUPAC: no longer '**phenethyl alcohol**' (P-29.6.3)



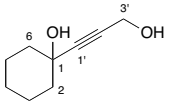
74 '3-phenylprop-2-en-1-ol'
- by (a)
- a conjunctive name is not possible because of the unsaturation in the chain
- formerly trivially '**cinnamyl alcohol**'



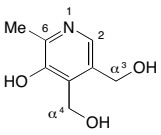
75 'α-phenylbenzenemethanol'
- by (a)
- conjunctive name
- IUPAC: no longer '**benzhydryl alcohol**' (P-29.6.3); trivially '**benzhydrol**'



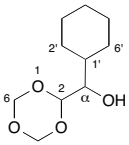
76 'α-ethenylcyclohexanepropanol'
- by (a)
- conjunctive name



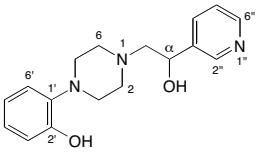
77 '1-(3-hydroxyprop-1-yn-1-yl)cyclohexanol'
- by (a)
- a conjunctive name is not possible because of the unsaturation in the chain



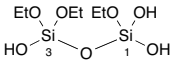
78 '5-hydroxy-6-methylpyridine-3,4-dimethanol'
- by (a)
- conjunctive name
- trivially '**pyridoxine**' or '**pyridoxol**', a '**vitamin B_6**'



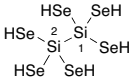
79 'α-cyclohexyl-1,3,5-trioxane-2-methanol'
- by (a)
- conjunctive name
- heterocycle > carbocycle



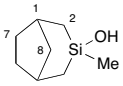
80 '4-(2-hydroxyphenyl)-α-pyridin-3-ylpiperazine-1-ethanol'
- by (a)
- conjunctive name



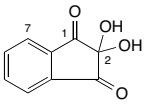
81 '1,3,3-triethoxydisiloxane-1,1,3-triol'
by (a)



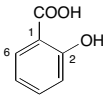
82 'disilane-1,1,1,2,2,2-hexaselenol'
by (a)



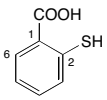
83 '3-methyl-3-silabicyclo[3.2.1]octan-3-ol'
by (a)



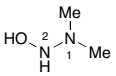
84 '2,2-dihydroxy-1*H*-indene-1,3(2*H*)-dione'
- by (a)
- indicated H atom by (h) of *§ A.5*, 'added' indicated H atom by (i_2) of *§ A.5*
- trivially '**ninhydrin**'



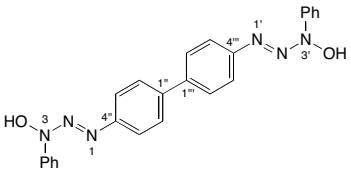
85 '2-hydroxybenzoic acid'
- by (a)
- trivially '**salicylic acid**'



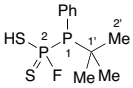
86 '2-mercaptobenzoic acid'
- by (a)
- trivially '**thiosalicylic acid**'



87 '2-hydroxy-1,1-dimethylhydrazine'
by (b)

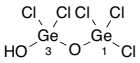


88 '1,1′-[1,1′-biphenyl]-4,4′-diylbis[3-hydroxy-3-phenyltriaz-1-ene]'
- by (b)
- multiplicative name

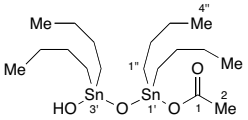


89 '1-(1,1-dimethylethyl)-2-fluoro-2-mercapto-1-phenyl~diphosphine 2-sulfide'
- by (b)
- additive name (=S at P^{III}); cf. (d) of *§ 6.20*

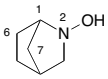
90 'hydroxytrimethylplumbane'
by (b)



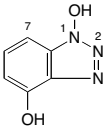
91 '1,1,1,3,3-pentachloro-3-hydroxydigermoxane'
by (b)



92 'acetic acid 1,1,3,3-tetrabutyl-3-hydroxydistannoxan-1-yl ester'/'1,1,3,3-tetrabutyl-3-hydroxydistannoxan-1-yl acetate'
- by (c)
- ester; see ester definition in (b_0) and (c) of *§ 6.14*, i.e., ester of a common acid and a nontraditional alcohol

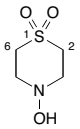


93 '2-hydroxy-2-azabicyclo[2.2.1]heptane'
by (b)

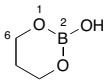


94 '1-hydroxy-1*H*-benzotriazol-4-ol'
- by (b)
- indicated H atom by (a) and (d) of *§ A.5*

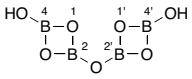
95 '1-hydroxy-1*H*-pyrazole 2-oxide'
- by (b)
- additive name (=O at N^{III}); cf. (d) of *§ 6.20*
- indicated H atom by (a) and (d) of *§ A.5*



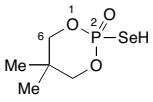
96 '4-hydroxythiomorpholine 1,1-dioxide'
- by (b)
- additive name (2 =O at S^{II}); cf. (d) of *§ 6.20*



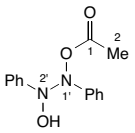
97 '2-hydroxy-1,3,2-dioxaborinane'
by (b)



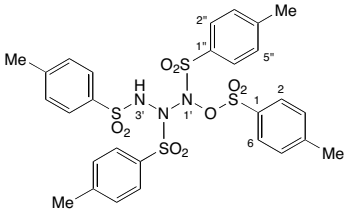
98 '2,2′-oxybis[4-hydroxy-1,3,2,4-dioxadiboretane]'
- by (b)
- multiplicative name



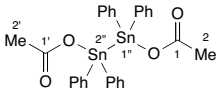
99 '5,5-dimethyl-2-selenyl-1,3,2-dioxaphosphorinane 2-oxide'
- by (b)
- additive name (=O at P^{III}); cf. (d) of *§ 6.20*



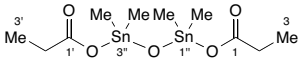
100 'acetic acid 2-hydroxy-1,2-diphenylhydrazinyl ester'/'2-hydroxy-1,2-diphenylhydrazinyl acetate'
- by (c)
- ester; see ester definition in (b_0) and (c) of *§ 6.14*, i.e., ester of a common acid and a nontraditional alcohol



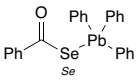
101 '4-methylbenzenesulfonic acid 1,2,3-tris[(4-methylphenyl)~sulfonyl]triazanyl ester'/'1,2,3-tris[(4-methylphenyl)sulfonyl]~triazanyl 4-methylbenzenesulfonate'
- by (c)
- ester; see ester definition in (b_0) and (c) of *§ 6.14*, i.e., ester of a common acid and a nontraditional alcohol



102 'acetic acid 1,1′-(1,1,2,2-tetraphenyldistannane-1,2-diyl ester'/'1,1′-(1,1,2,2-tetraphenyldistannane-1,2-diyl) bis[acetate]'
- by (c)
- ester; see ester definition in (b_0) and (c) of *§ 6.14*, i.e., ester of a common acid and a nontraditional alcohol

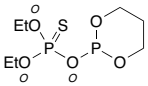


103 'propanoic acid 1,1′-(1,1,3,3-tetramethyldistannoxane-1,3-diyl) ester'/'1,1′-(1,1,3,3-tetramethyldistannoxane-1,3-diyl) bis[propanoate]'
- by (c)
- ester; see ester definition in (b_0) and (c) of *§ 6.14*, i.e., ester of a common acid and a nontraditional alcohol



104 'benzenecarboselenoic acid *Se*-(triphenylplumbyl) ester'/ '*Se*-(triphenylplumbyl) benzenecarboselenoate'

- by (c)
- ester; see ester definition in (b_0) and (c) of *§ 6.14*, i.e., ester of an exotic acid and a nontraditional alcohol



105 'phosphorothioic acid *O*-1,3,2-dioxaphosphorinan-2-yl *O,O*-diethyl ester'/ '*O*-1,3,2-dioxaphosphorinan-2-yl *O,O*-diethyl phosphorothioate'

- by (c)
- ester; see ester definition in (b_0) and (c) of *§ 6.14*, i.e., ester of a common acid and a nontraditional alcohol