

**Changes in the 2005 edition of the  
“Nomenclature of Organic Chemistry, 2005 edition”  
from the 1979 edition and the 1993 Guide**

## 1. Introduction

The 2005 edition of the “Nomenclature of Organic Chemistry, 2005 edition is based on the following:

- (a) The scope of the nomenclature of organic compounds is extended to include all elements of Groups 13, 14, 15, 16, and 17.
- (b) Substitutive nomenclature is the preferred method of nomenclature, except for anhydrides, esters and salts, acid halides and pseudohalides for which traditional functional class names are maintained. Substitutive nomenclature is based on the names of parent hydrides modified by suffixes and prefixes; parent hydrides can be modified by using skeletal replacement (‘a’) nomenclature and functional replacement nomenclature, and also by additive (for example, addition of hydrogen atoms or ions) and subtractive operations (for example, subtraction of hydrogen atoms or ions).
- (c) Generalized ‘ane’ nomenclature is recommended. Substitutive nomenclature is applied to each element of Groups 13, 14, 15, 16, and 17 having a fixed number of hydrogen atoms which are used as mononuclear or polynuclear parent hydrides in the way described for alkanes. The names ‘alumane’ is recommended for  $\text{AlH}_3$ , ‘gallane’ for  $\text{GaH}_3$ , ‘indigane’ for  $\text{InH}_3$ , and ‘thallane’ for  $\text{TlH}_3$ . Suffixes and prefixes are attached to any parent hydride in the same way that is recommended alkanes, for example ‘trisulfanecarboxylic acid’ for  $\text{HSSS-COOH}$ , ‘trimethylsilanol’ for  $(\text{CH}_3)_3\text{Si-OH}$ , ‘phenylstibanone’ for  $\text{C}_6\text{H}_5\text{Sb=O}$ , and trimethylalumane for  $(\text{CH}_3)_3\text{Al}$ .
- (d) Some well entrenched and widely used trivial names are maintained to identify the parent hydrides: ‘methane’, ‘ethane’, ‘propane’ and ‘butane’ for alkanes and names of monocyclic and polycyclic carbocycles and heterocycles used to create all polycyclic fused rings. Retained names of functional parents and characteristic groups have been reduced as has been done with each succeeding edition of the “Nomenclature of Organic Chemistry”.

## 2. Specific changes.

### (a) Chapter P-1

- (1) The **list of multiplying prefixes** has been completed from 11 to 9999. The prefixes are formed by changing the ending ‘a’ of the basic numerical prefixes into ‘i’, for example ‘undeci’ for 11, ‘hexadeci’ for 16, and ‘tetraconti’ for 40 (see P-14.2.3).

(2) **Numbering.** Three changes have been made to the 1979 recommendations:

- (a) **heteroatoms in chains** are now considered as part of the parent hydride; as such they have seniority over suffixes for numbering (see P-14.4; see also P-15.4.3); this change makes 'a' terms nondetachable in skeletal replacement in chains, rings and ring systems [See (c) below]
- (b) **hydro/dehydro prefixes** are now classified as detachable prefixes but are not included in the category of alphabetized detachable prefixes (see P-14.4; see also P-15.1.3.2, P-31.2, P-58.2); this change from nondetachable to detachable status makes the subtraction of hydrogen atoms denoted by 'ene' and 'yne' endings or 'dehydro' prefix, and addition of hydrogen atoms denoted by 'hydro' prefix in the same category with respect to numbering nomenclatural features in the construction of names. [(See( c) below]
- (c) When necessary, **numbering of various nomenclatural features** is achieved by considering, in the following decreasing order of seniority, until a decision is reached (see P-58.2):
  - (i) fixed numbering, as for naphthalene, bicyclo[2.2.2]octane;
  - (ii) **heteroatoms in heterocycles and acyclic parent structures;**
  - (iii) indicated hydrogen [for unsubstituted compounds, a higher locant may be needed at another position to provide for a substituent suffix in accordance with structural feature (iv) below];
  - (iv) principal group named as suffix;
  - (v) added hydrogen (consistent with the structure of the compound and in accordance with further substitution);
  - (vi) **saturation ('hydro/dehydro' prefixes or unaturation ('ene/yne' endings)**
  - (vii) substituents named as prefixes (low locants are allocated for substituents regardless of kind, then, if necessary, in the order of citation in the name)

(3) **Multiplicative nomenclature** (P-15.3.). Multiplicative nomenclature has been reserved for naming compounds having characteristic groups expressed as suffixes or implied by a retained name, and for heterocyclic parent hydrides. It is now extended to cyclic structures with or without characteristic groups; chains composed only of carbon

atoms are excluded from this type of nomenclature; the traditional approach based on substitutive nomenclature is recommended. The system has also been expanded by allowing substitution on the central unit of a multiplying group and the use of nonsymmetrical central units under specific conditions.

- (4) In **skeletal replacement ('a') nomenclature** the chain had to be terminated by carbon atoms (Rule R-2.2.3.1 in the 1993 Guide); now, the following heteroatoms: P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, and Tl can terminate the chain (P-15.4.3.2.3)

**(b) Chapter P-2 Parent hydrides**

- (1) **Hantzsch-Widman system** (P-22.2.2). The elements aluminium, gallium, indium and thallium are now included in the system and mercury is no longer included.
- (2) **von Baeyer nomenclature.** Rule A-32.23 in the 1979 Recommendations (ref. 1) and Rule R-2.4.2.2 in the 1993 Recommendations (ref. 2) have been replaced by P-23.2.5.2: 'After the main ring and main bridge have been numbered, the independent secondary bridge is numbered continuing from the higher numbered bridgehead of the main ring' and Rule P-23.2.6.3 on secondary bridges.

**(3) Spiro nomenclature.**

- (a) After due consideration, the (former) Commission on Nomenclature of Organic Chemistry opted to maintain alphabetical order for naming spiro compounds composed of different components rather than an ordering based on the seniority order of rings and ring systems (P-24.5.1)
- (b) **P-24.5.2.** 'Monospiro compounds with different components at least one being polycyclic and at least one requiring the use of skeletal replacement ('a') nomenclature are named as in P-24.5.1, then, the skeletal replacement ('a') prefixes are introduced and cited before the spiro term'. This is a change from the publication given in ref. 8 (see SP-4.1) in which the skeletal replacement ('a') prefixes were kept within the component ring system.
- (c) **Polyhelicenes** (P-25.1.2.6). The definition of a polyhelicene has been changed. The series begins with 6 rings and not five rings as indicated in the 1993 Guide (R-2.4.1.3.6 in ref. 2) and in the Glossary of Class Names. A further change related to the orientation and numbering recommended in the comprehensive fused ring nomenclature document 'Nomenclature of Fused and Bridged Fused Systems' (ref. 4) is included. This new orientation and numbering are presented in Section P-25.3.3.

**(4) Fusion nomenclature** (P-25.3.1.3)

- (a) **General Principles.** In the 1998 Recommendations (ref. 4), the requirement that at least two rings of five or more members must be present for the application of fusion nomenclature contained in the 1979 Recommendations

(ref. 1), was removed. For selection of preferred IUPAC names, however, this requirement is reinstated in the 2005 recommendations. However, in general nomenclature, the fusion system can be applied equally to smaller rings, as in 'cyclobutabenzene'.

- (b) **Elision of vowels.** In the previous 1979 rules (Rule A-21.4, ref. 1) the elision of the final letter 'o' of acenaphtho, benzo, naphtho and perylo and the final letter 'a' of the monocyclic prefixes cyclopropa, cyclobuta, etc. was recommended. In ref. 4 (FR-4.7) and in these 2005 recommendations this elision is no longer recommended, hence benzo[g]isoquinoline rather than benz[g]isoquinoline.[See also P-16.6.2 f)]
- (c) **Numbering of interior carbon atoms** (P-25.3.3.3). A major change to the rule for interior numbering interior carbon atoms is now recommended (see FR-5.5.2 in ref. 4). Interior atoms are numbered by identifying the minimum number of bonds linking them to a peripheral atom. The locant for the interior atom is that of the peripheral atom with a superscript number corresponding to the number of bonds between the two atoms. The previous 1979 rule (Rule A-22.2 in ref. 1) recommended that interior atoms follow the highest numbered peripheral atom adding Roman letters in sequence to the appropriate peripheral number.
- (6) **Bridged fused ring systems** (P-25.4.2.1.4) Names of divalent acyclic homogeneous heteroatom bridge have been changed with respect to the parent hydride and the use of 'epi'. For example 'epithio', for -S-, in the 1993 Recommendations (ref. 2) is now 'sulfano'; the group -NHNH-, formerly 'diazano', is now 'epidiazano'.
- (7) **Phane nomenclature** (P-26) and **fullerene nomenclature** (see P-27) are now included in the chapter discussing the various nomenclatures for parent hydrides.
- (8) **Ring assemblies** (P-28)
- (a) **Numbering.** A new numbering system is recommended for ring assemblies composed of more than two rings or ring systems. The elimination of primed locants is intended to improve the perception of the relationship between structures and names. The new system is analogous to that recommended in phane nomenclature. For instance, two alternative names are 1,1',2',1''-tercyclopropane and 1<sup>1</sup>,2<sup>1</sup>,2<sup>2</sup>,3<sup>1</sup>-tercyclopropane, where the primary locants 1,2,3 correspond to the three rings of the assembly, and the superscript locants to the locants of the points of attachment of these three rings.
- (b) **Citation of indicated hydrogen atoms** (P-28.4). The citation of indicated hydrogen, if needed, at the front of the name of a ring assembly is a change from previous practice where indicated hydrogen was kept within the name of the individual ring, for example, 2,2'-bi-2*H*-pyran is now 2*H*,2*H'*-2,2'-bipyran.

The advantages of this method become more obvious when naming derivatives of ketones or divalent substituent groups.

(9) **Substituent groups.**(P-29)

- (a) The specific method for naming substituent groups by replacing the ending 'ane' by the suffix 'yl' (P-29.2.1), as in methyl, is no longer recommended for naming substituent groups of borane. Thus, the name is 'boranyl', not 'boryl', for  $\text{H}_2\text{B}-$ .
- (b) When names are formed by the specific method described in P-29.2.1, names generated by adding the suffix 'yl' to the name of the parent hydride, for example 'methanyl', are not recommended (P-29.3.1).
- (c) When free valences are not at the end of the longest chain, the general method (P-29.3.1) is preferred over retained names or compound names, for example, propan-2-yl is the preferred name and not isopropyl or 1-methylethyl.

(c) **Chapter P-3** Characteristic (functional) groups

- (1) **Unsaturated spiro compounds** Unsaturation in a spiro ring system with one or more components named by the von Baeyer system is indicated by the endings 'ene', 'diene', etc. They are cited after the last bracket of the spiro name; only the final letter 'e' of the saturated hydrocarbon name is elided if followed by a vowel. If there is a choice, low locants are assigned, in order, to spiro junction(s), heteroatoms and double bonds. This is a change from the Guide (ref. 2; see ref. 7), for example: 2,2'-spirobi[bicycle[2.2.1]heptan]-5-ene.
- (2) **Suffixes.** The suffix 'peroxol' for  $-\text{OOH}$  has been added to the list of basic suffixes. It is modified by functional replacement generating the suffixes '-OS-thioperoxol' for  $-\text{OSH}$  and '-SO-thioperoxol' for  $-\text{SOH}$ . The suffix 'sulfenic acid' for  $-\text{SOH}$  has been abandoned in the 1993 Recommendations (see ref. 2).

(d) **Chapter P-4.** Rules for name construction

- (1) The partial seniority order of classes presented in the Guide (see R-4.1, ref. 2) has been completed by the inclusion of all functions and elements; it is discussed in P-41.
- (2) A complete order of **seniority for acids** (carboxylic acids and inorganic acids having retained names) is presented in P-42. For consistency in the names of polynuclear oxoacids, the numerical infix 'di' has been uniformly used in names of dinuclear 'hypo' acids, for example, hypodiphosphorous acid, rather than hypophosphorous acid.
- (3) A complete order of **seniority of suffixes** and suffixes modified by functional replacement is presented in P-43.

- (4) The seniority order of **parent structures** (rings, ring systems and chains) is presented in P-44. The revision leads to a major change. In this document, it is recommended to invert the traditional order of seniority between unsaturation and length in the case of acyclic compounds; thus, the first criterion is concerned with the length of the chain and unsaturation is second to length. This change gives seniority to parent hydrides rather than to modified parent hydrides (see P-44.3 and also P-32.1.1)
- (5) Chapter P-4 also includes a section on the principal chain in substituent groups (P-45) and substitution rules for parent structures with retained names (P-46).

**(e) Chapter P-6**

- (1) **Pseudoketones** (P-64.5.2.1 and P-66.1.2.3) have the generic formula X-CO-C or X-CO-Y, where X and Y are heteroatoms and the ketone group is the principal characteristic group. Preferred IUPAC names are formed by using the suffix 'one'. For example: 1-(trimethylsilyl)ethan-1-one for  $(\text{CH}_3)_3\text{Si-CO-CH}_3$ . Hidden amides are named as pseudoketones, for example, 1-(piperidin-1-yl)propan-1-one for  $\text{C}_5\text{H}_{10}\text{N-CO-CH}_2\text{-CH}_3$ .
- (2) **Heterones** are compounds having an oxygen atom formally doubly bonded to a heteroatom, for example dimethylsilanone for  $(\text{CH}_3)_2\text{Si=O}$  (see P-64.4).
- (3) **Acyl groups** (P-65.1.7). Traditional names of acyl groups are maintained, but systematic substitutive names are recommended for acyl groups modified by functional replacement. For example, 'acetyl' for  $\text{CH}_3\text{-CO-}$  but 'ethanethioyl' and 'ethanimidoyl' for  $\text{CH}_3\text{-CS-}$  and  $\text{CH}_3\text{-C(=NH)-}$ , respectively (oxalic acid is an exception, see P-65.2.3).
- (4) **Acyl substituent group names** are derived from the names of the acids and not by concatenation, for example, propane-1-sulfonyl and not propylsulfonyl (P-65.4.1)
- (5) **Preferred names for acyl groups** derived from carbonic acid and the N, P, As, and Sb inorganic oxo acids, are formed from the names of acids, modified or not by functional replacement nomenclature, for example: carbonochloridoyl, for  $\text{-CO-Cl}$ , derived from carbonochloridic acid,  $\text{HO-CO-Cl}$  (see P-65.2.1.5); phosphorochloridocyanidoyl, for  $\text{-P(=O)Cl(CN)}$ , from  $\text{HO-P(=O)Cl(CN)}$ , phosphorochloridocyanidic acid (see P-67.1.4.1.1)
- (6) **Pseudoesters** (P-65.6.3.4). Compounds of the type  $\text{R-CO-O-E(R')}_3$  are generically called 'pseudoesters' and named as esters, for example,  $\text{CH}_3\text{-CO-O-Si(CH}_3)_3$  is named trimethylsilyl acetate.
- (7) **Polyanhydrides** (P-65.7.7). The nomenclature of polyanhydrides has been fully developed, for example 'diacetic butanedioic dianhydride' for  $\text{CH}_3\text{-CO-O-CO-CH}_2\text{-CH}_2\text{-CO-O-CO-CH}_3$ .
- (8) **Organic derivatives of inorganic acids** (P-67) have been fully systematized, based on retained names of inorganic acids (for example, 'phosphoric acid') and systematic substitutive names.

- (9) **Suffixes** are recommended to name appropriate compounds of Group 13 (see P-68.1.5.1), Group 14 (see P-68.2.5), Group 15 (see P-68.3.2.3.1 and P-68.3.3), Group 16 (see P-68.4.1.1 and P-68.4.2.2) and Group 17 (see P-68.5.1).
- (10) **Organic derivatives** of borane,  $\text{BH}_3$ ; alumane,  $\text{AlH}_3$ ; gallane,  $\text{GaH}_3$ ; indigane,  $\text{InH}_3$ ; and thallane,  $\text{TlH}_3$ , are described in Section P-68.1. Organic derivatives of trioxidane,  $\text{HOOOH}$ , trisulfane,  $\text{HSSSH}$ , etc. and their polynuclear homologues are described in P-68.4. Organic derivatives of hydrides of Group 17 with bonding numbers higher than 1 are described in Section P-68.5.
- (11) **Organometallic compounds.** The contribution of the nomenclature of organic compounds to the nomenclature of organometallic compounds has been discussed and exemplified, with extension of the substitutive nomenclature applied to Groups 13 through 17 to metals of Groups 3 to 12.

**(f) Chapter P-7.**

- (1) **Nomenclature for radicals, anions, cations, and radical ions** previously published (ref. 3) has been expanded to include delocalised systems including 1,2- and 1-3-dipolar ions and nonclassical structures. Criteria to determine the seniority order of 'ide' and 'uide' anions is described in P-72.5.1; seniority order for 'ium' and 'ylium' cations are described in P-73.7. Criteria to choose radical and ionic parent structures are described in P-71.7 for radical parent structures, P-72.7 for anionic parent structures and P-73.7 for cationic parent structures.

**(g) Chapter P-9** The section on **configuration** has been expanded to cover the CIP system for prioritizing atoms and groups (see P-91) and the CIP stereodescriptors for describing chirality centers, axes and planes (see P-92).

**(h) Chapter P-10** Section F (see ref. 1) has been expanded to cover carbohydrates, amino acids and peptides, cyclitols, nucleosides, nucleotides, and lipids.