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Division VIII Chemical Nomenclature and Structure Representation Division

Nomenclature of Organic Chemistry. IUPAC Recommendations and Preferred Names 2013.

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PREFACE

This edition of the *Nomenclature of Organic Chemistry* follows the 1993 publication of the *Guide to IUPAC Nomenclature of Organic Compounds* by the International Union of Pure and Applied Chemistry (IUPAC). The International Union of Pure and Applied Chemistry has the responsibility to establish rules for systematic nomenclature. The Rules for Organic Chemistry were first issued in Geneva in 1892. They were followed by the Liége Rules in 1930 and the IUPAC rules in 1957 (Sections A and B), 1969 (Sections A, B, and C) codified as the Blue Book, and 1979 (Sections A, B, C, D, E, F, and H). The 1993 Guide recognized the necessity to propose to the chemical community the so called ‘preferred IUPAC name’, not to say the ‘unique name’. The explosion of information justifies this new approach in the revision of the principles, rules, and conventions of the nomenclature of organic compounds. Preferred IUPAC names, known under the friendly acronym PIN, are also important in legal situations, with manifestations in patents, export-import regulations, health and safety information, and communications in environmental sciences and their legal implications.

The work for this edition began in 1992 at the time the 1993 Guide was in press under the expert guidance of the Commission on Nomenclature of Organic Chemistry (CNOC). The general format of the Guide was maintained. The principal objective was to maintain continuity and consistency. Continuity meant that substitutive nomenclature was maintained as the principal nomenclature to name organic compounds based on the concepts of parent hydrides and of different hierarchical orders: order of classes, order of seniority of suffixes, seniority order for rings and ring systems, and seniority order for chains (the principal chain). Consistency was to consider the hydrides of elements of Groups 13, 14, 15, 16, and 17 as parent hydrides in substitutive nomenclature and to treat equally carbon atoms and heteroatoms. To achieve this goal, the names of the hydrides of heteroatoms are names ending in ‘ane’, for example ‘phosphane’ for PH₃ and ‘silane’ for SiH₄. As they are chosen amongst several (inorganic) names, for instance ‘sulfane’ and ‘hydrogen sulfide’ for H₂S, these names are called ‘preselected names’; the decision to accept them as ‘preferred IUPAC names’ will be made later. Preselected names generate preselected prefixes and suffixes, for example ‘sulfanyl’ and ‘sulfanylidene’ for –SH and =S, respectively, which are used in substitutive nomenclature, as are preferred prefixes and suffixes, such as ‘methyl’, –CH₃, and ‘phenyl’, –C₆H₅.

Several changes from previous rules were needed to achieve systematization and consistency in constructing names. To facilitate the understanding and use of the preferred IUPAC name system, these changes are explained and highlighted in boxes each and every time they appear in Chapters P-1 through P-8. In Chapter P-6, full systematization has been applied to the formation of prefixes of substituent and functional groups.

It is hoped that the systematization provided by the strict application of the rules will be widely understood and accepted. Preferred IUPAC names are easy to be selected. It is however inevitable that some ambiguities and unsuspected difficulties will be encountered. Task forces will be established to rapidly answer questions, give guidance to authors and ensure the homogeneity of the system. Computerized nomenclature should help in maintaining this homogeneity and in making sure that further progress will be firmly consistent with it.

It is important to reiterate that nomenclature is here to serve a number of purposes: oral communication, commercial and industrial development, written scientific communication, etc. As has been many times, the prime aim of IUPAC nomenclature is clarity and the construction of unambiguous names; there must be absolute correspondence between structure and name, and vice versa between name and structure. Preferred IUPAC names are here today to serve a special purpose; they are not imposed to the chemical and scientific community. The rules set out here express the firm belief of the former Commission on Nomenclature for Organic Chemistry, now that of the IUPAC Chemical Nomenclature and Structure Representation Division, as to the best system of nomenclature, for present specific purposes and for future developments.

ACKNOWLEDGMENTS

Many thanks are due to a large number of contributors. The shaping of the project and supervision over the early draft stages was done by members of the IUPAC Commission on Nomenclature of Organic Chemistry from 1993 until its demise in 2001. The membership of the Commission on Nomenclature of Organic Chemistry from 1993 through 2001 is given above. In 2002, responsibility for the project then passed to the IUPAC Division of Chemical Nomenclature and Structure Representation who followed its development through 2013. The membership of the Division Committee from 2002 through 2013 is also given above. It is also in order to thank all members of the Division Committee and other colleagues who submitted general or specific comments and/or participated in discussions, either by correspondence, or by means of the IUPAC Division VIII Webboard located on the RSC web site during the preparation of the first full draft in 2004 on which many comments and suggestions were received. Many sincere thanks must be given to Alan McNaught who, along with the authors, spent many days reviewing the hundreds of comments and suggestions received on the 2004 draft which resulted in a revised draft in 2010 which was again posted for review on the Division VIII Webboard. Many comments made on the 2010 draft were simply repeats of the comments made for the 2004 draft. Significant and useful comments came from Jonathan Brecher, Ursula Bünzli-Trepp, Ture Damhus, Ted Godly, Harry Gotlieb, Richard Hartshorn, Karl-Heinz Hellwich, Bernardo Herold, J. Kahovec, L. Maat, Paulina Mata, József Nyitrai, Arthur Maximenko, Andrey Yerin, Richard Cammack, Hal Dixon, Gernot Eller, Rita Hoyos de Rossi, Jan Reedijk, Alexander Senning, L. Salvatella, Roger Sayle, and Hervé Schepers leading finally to these 2013 recommendations. We must also thank Marcus Ennis who spent weeks giving the 2013 draft a complete edit for errors in both language and chemistry.

CHANGES FROM THE 1979 EDITION, THE 1993 GUIDE, AND OFFICIAL PUBLICATIONS FROM 1993 THROUGH 2002 INCLUDED IN THE 2013 EDITION OF THE IUPAC NOMENCLATURE OF ORGANIC CHEMISTRY, 2013 EDITION

1. Scope of the recommendations in the 2013 edition

(a) The elements Al, Ga, In, and Tl are added to the elements that were included in the recommendations in the 1979 edition (ref. 1) and the 1993 Guide (ref. 2)

2. Skeletal replacement ('a') nomenclature

(a) Heteroatoms in chains subject to skeletal replacement ('a') nomenclature are considered to be an integral part of the parent hydride and as nondetachable prefixes they have seniority over suffixes for numbering; thus, heteroacyclic chains subject to skeletal replacement ('a') nomenclature are now treated the same as heterocyclic rings.

(b) The heteroatoms P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, and Tl can now terminate a heteroacyclic chain that is subject to skeletal replacement ('a') nomenclature; in previous recommendations, a heteroacyclic chain that is subject to skeletal replacement ('a') nomenclature had to terminate with carbon atoms.

(c) Skeletal replacement ('a') prefixes ending in 'ata', for example 'borata', are no longer recognized.

(d) Groups of heteroatoms having a single multivalent name are considered as a unit; hence the term 'heterounit' includes both heteroatoms and such heteroatom groups. Such heteroatom groups were not considered as a single heterounit in previous recommendations.

(e) Adapting skeletal replacement ('a') prefixes for elements of Groups 1-12 for use in skeletal replacement nomenclature is a major change even though names for such organometallic compounds involving these elements are only preselected at this time.

3. Substitutive nomenclature

- (a) 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 hydride names can be modified by using skeletal replacement ('a') nomenclature and functional replacement nomenclature, and also by additive operations (for example, addition of hydrogen atoms or ions) and subtractive operations (for example, subtraction of hydrogen atoms or ions).
- (b) Generalized 'ane' nomenclature is recommended for preferred IUPAC names. 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 mono-nuclear or polynuclear parent hydrides in the same way as described for alkanes. Recommended names are 'alumane' for AlH_3 , 'gallane' for GaH_3 , 'indigane' for InH_3 , and 'thallane' for ThH_3 . Suffixes and prefixes are attached in the same way as for alkanes, for example 'trisulfanecarboxylic acid' for 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 $(\text{CH}_3)_3\text{Al}$.
- (c) 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. The number of retained names for functional parents and characteristic groups has been reduced, as has been done with each succeeding edition of the IUPAC "Nomenclature of Organic Chemistry".
- (d) Toluene and xylene are retained preferred IUPAC names, but are not freely substitutable. Toluene is substitutable under certain conditions only in general nomenclature. Mesitylene is a retained name but only for general nomenclature and cannot be substituted. In the 1993 Guide (ref. 2), these parent hydrides were also retained but only limited substitution was allowed.
- (e) Hydrazidines are named systematically as '-hydrazonohydrazides' and not as hydrazones of the corresponding hydrazides as in the 1979 recommendations.
- (f) Oximes are named substitutively as '*N*-hydroxy' derivatives of imines and not by functional class nomenclature as in previous recommendations.
- (g) Hydrazones and azines are named substitutively as 'ylidene' derivatives of hydrazine and not by functional class nomenclature as in previous recommendations.

4. Multiplicative nomenclature

- (a) Multiplicative nomenclature is now extended to cyclic structures with or without characteristic groups; chains composed only of carbon atoms continue to be excluded. In past recommendations multiplicative nomenclature was limited to compounds having characteristic groups expressed as suffixes or implied by a retained name and to heterocyclic parent hydrides. The system now has also been expanded to allow substitution on the central unit of a multiplying group and the use of nonsymmetrical central units under specific conditions.
- (b) In these recommendations, all substituent groups, including the principal characteristic groups must be identical and have the same locant in order to construct a multiplicative name. This is a change from earlier recommendations where such locants did not need to be identical.

5. Hydro or dehydro prefixes are introduced in names by an additive or subtractive operation and are now classified as detachable prefixes but are not included in the category of alphabetized detachable prefixes which describe substitution. In names, they occupy a permanent place between the nondetachable prefixes attached just before the parent structure and the alphabetizable detachable prefixes describing substitution. The change from nondetachable to nonalphabetizable detachable prefixes gives 'hydro' and 'dehydro' prefixes the same status with respect to numbering nomenclatural features in the construction of names as the subtraction of hydrogen atoms denoted by 'ene' and 'yne' endings. In names, the prefix 'dehydro' precedes the prefix 'hydro', when both are present. Simple numerical terms, such as 'di-', 'tetra-', etc., are used with 'hydro' and 'dehydro' prefixes. Hydro or dehydro prefixes are numbered according to the principle of lowest locants, in accord with the numbering of the parent hydride and after priority has been given to indicated hydrogen, added indicated hydrogen, and suffixes, when present, as specified in the general rules for numbering.

6. Suffixes

- (a) The suffix 'peroxol', for $-\text{OOH}$, has been added to the list of basic suffixes and is modified by functional replacement nomenclature, generating the suffixes ' $-\text{OS-} \text{thioperoxol}$ ' for $-\text{OSH}$, and ' $-\text{SO-} \text{thioperoxol}$ ' for $-\text{SOH}$. The suffix 'sulfenic acid', for $-\text{SOH}$, was abandoned in the 1993 Recommendations.
- (b) Systematic suffixes, for example methanimidic acid, imidic acids, hydrazonic acids, peroxyacidic acids, and chalcogen analogues of monocarboxylic acids, are changes for formic acid, acetic acid, benzoic acid, and oxalic acid.

(c) Suffixes are now used in accordance with the seniority of classes (see P-41) for germanium, tin and lead compounds which is a change from the previous recommendations where only prefixes were used.

(d) The suffix ‘-hydrazide’ rather than ‘-ohydrazide’ used in previous recommendations is used for naming acyclic hydrazides in accordance with the general use of suffixes added to names of parent hydrides, for example pentanehydrazide for $\text{CH}_3\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{-CO-NH-NH}_2$, not pentanohydrazide.

7. Prefixes

(a) The preselected prefix ‘nitrilo’ is used only when the three bonds from nitrogen are attached to different atoms; it is no longer used for the structure $-\text{N}=$, which now has the preselected prefix ‘azanylylidene’.

(b) The preselected prefix ‘azanediyl’ derived from the preselected parent hydride name ‘azane’ is now used for the multiplicative substituent group $-\text{NH}-$; the preselected prefix ‘imino’ is used only to designate $=\text{NH}$ as a substituent.

(c) Prefixes derived from borane are now named only by the general method [method (2) in P-29.2], namely ‘boranyl’, ‘boranylidene’, and ‘boranylidyne’, rather than by the method used for the elements of Group 4 [method (1) in P-29.2]; the prefix ‘boryl’ is discarded.

(d) The preselected prefixes ‘sulfanylidene’, ‘selanylidene’, and ‘tellanylidene’, for $=\text{S}$, $=\text{Se}$, and $=\text{Te}$ as substituents, respectively, are used in preferred IUPAC names to designate the chalcogen analogues of the preselected prefix ‘oxo’. The prefixes ‘thioxo’, ‘selenoxo’, and ‘telluroxo’ derived by functional replacement nomenclature may be used in general nomenclature.

(e) Simple substitutive acyl prefixes directly derived from the name of a ‘sulfonic acid’, ‘sulfinic acid’, and their chalcogen analogues as in ‘benzenesulfonyl’ and ‘benzenetellurodithietyl’ are used in preferred IUPAC names and not prefixes formed by concatenation, for example ‘phenylsulfonyl’, which can be used in general nomenclature.

(f) The prefixes ‘ureido’ and ‘ureylene’ are not used in IUPAC names. The prefixes ‘carbamoylamino’ and ‘carbonylbis(azanediyl)’, respectively, are recommended for preferred IUPAC names and in general nomenclature.

(g) The prefix ‘guanidino’ is no longer acceptable in preferred IUPAC names but may be used in general nomenclature; the preferred prefix is ‘carbamimidoylamino’.

(h) The prefix ‘amidino’ is no longer acceptable in IUPAC names; the preferred prefix is ‘carbamimidoyl’.

(i) The prefix ‘*aci*-nitro’ for HO-N(O)= is no longer acceptable for preferred IUPAC names; it was discontinued in the 1993 Guide (ref. 2). The preferred prefix is ‘hydroxy(oxo)- λ^5 -azanylidene’; the prefix recommended in the 1993 Guide (ref. 2) ‘hydroxynitroaryl’ is not acceptable in the context of these recommendations where two free valences must be expressed by the correct ‘ylidene’ or ‘diyl’ type.

(j) Preselected prefixes derived from the preselected parent hydride hydrazine are now formed systematically from hydrazine: ‘hydrazinyl’ for $\text{H}_2\text{N-NH-}$; ‘hydrazinylidene’ for $\text{H}_2\text{N-N=}$; ‘hydrazinediylylidene’ for $=\text{N-N=}$; and hydrazine-1,2-diyl for $-\text{NH-NH-}$. The prefixes ‘hydrazino’, ‘hydrazono’, ‘azino’ and ‘hydrazo’, respectively, are no longer acceptable, even for general nomenclature.

(k) The prefixes ‘benzyl’, ‘benzylidene’, and ‘benzylidyne’ cannot be substituted for preferred IUPAC names, although for general nomenclature restricted substitution is permitted (see P-29.6.2). In the 1993 Guide (ref. 2), these prefixes could only be substituted on the ring.

(l) Preferred prefixes derived from ‘triazane’ and ‘tetraazane’ are named systematically as hydrocarbons are named, for example ‘triazan-1-yl’, ‘tetraazan-2-yl’. The prefixes ‘triazano’ and ‘tetraazano’ previously used for ‘triazan-1-yl’ and ‘tetraazan-1-yl’ and also as bridge prefixes must not be used even though as bridge prefixes they are now named ‘epitriazano’, etc.

(m) Acyl prefixes formed from acyclic parent hydrocarbons and prefixes such as ‘oxo’, ‘thioxo’, ‘sulfanylidene’, and ‘imino’, for example, ‘1-oxopropyl’ are not preferred prefixes for preferred IUPAC names, but can be used in general nomenclature; they are used in CAS index nomenclature.

(n) Functional replacement analogues of formic, acetic, benzoic, and oxalic acids and acyl prefixes derived from them are named systematically, for example, methanimidic acid not formimidic acid, benzenecarboximidoyl not benzimidoyl, and ethanediperoxoic acid not diperoxyxallic acid.

(o) Simple prefixes are used before prefixes beginning with a multiplicative prefix where ‘bis-’, ‘tris-’, etc., were used in previous recommendations.

(p) The $-\text{N}=\text{C=O}$ group, its chalcogen analogues, and the $-\text{NC}$ group have been added to the list of characteristic groups that are always cited as prefixes in substitutive nomenclature. Thus, when attached to a parent hydride these groups are named substitutively using the prefixes ‘isocyanato’, ‘isothiocyanato’, ‘isoselenocyanato’,

‘isotellurocyanato’, and ‘isocyano’, respectively, in preferred IUPAC names. In previous recommendations they were also expressed by functional class nomenclature.

(q) The potentially ambiguous names ‘fulminate’ and ‘fulminato’ are discarded in favor of systematic names.

8. Locants

(a) Superscript arabic numbers are now used to differentiate the nitrogen atoms of symmetrical geminal diamines, diimines, diamides, diimidamides, diamidines, dihydrazonamides and/or imidohydrazides, diamidrazones, and dihydrazonohydrazides and for nitrogen atoms that are not a part of the main chain in names of imidodi-, polyimido-, and di- and polynuclear acid chains, including di- and polycarbonic acids. Primes ('), double primes ("), triple primes (""), etc., were used in previous recommendations

(b) Superscript arabic numbers are now used to locate chalcogen atoms of di- and polynuclear oxoacids, including di- and polycarboic acids. Online arabic numbers were used in previous recommendations.

(c) Numerical locants are no longer used in IUPAC names for urea, thiourea, condensed ureas, semicarbazide, semicarbazone, and the cation uronium.

(d) The locants N and N' are used for the $-NH_2$ and $=NH$ group of amidines, respectively rather than the locants N^1 and N^2 which were used in the 1979 recommendations (ref. 1).

9. Acyclic systems

(a) In a homogeneous acyclic structure the length of the chain is now preferred to unsaturation for choosing the preferred parent acyclic chain and the preferred parent chain of a preferred prefix; this is the reverse of these criteria from those in previous recommendations.

(b) The nomenclature for an $a(ba)_x$ heteroacyclic chain does not apply when the ‘b’ element is nitrogen or carbon; this is a change from the 1993 Guide (ref. 2) where the ‘amine’ characteristic group present in such a system was not recognized and carbon was not excluded as a ‘b’ element.

10. Hantzsch-Widman system

(a) The final ‘e’ in Hantzsch-Widman names is required in preferred IUPAC names; it is still optional in general nomenclature. In the 1979 Rules (ref. 1), the final ‘e’ of a Hantzsch-Widman name was omitted when there was no nitrogen in the ring; in the 1993 Guide (ref. 2) the final ‘e’ was optional.

(b) The element mercury is removed from the Hantzsch-Widman system.

(c) Adapting the elements of Groups 1-12 to the principles of the Hantzsch-Widman nomenclature system is a major change, even though organometallic compounds involving these elements are only preselected at this time.

11. Polycyclic ring systems

(a) The use of indicated hydrogen (see P-14.7.1) for bridged fused ring systems, spiro ring systems (see P-24.3.2), and ring assemblies (see P-28.2.3) is now implemented in the same way as for mancude monocyclic and polycyclic fused ring systems (see P-25.7.1.1). The operation is simple and uniformly applied. The skeletal graph is first drawn and heteroatoms are added. Then, the maximum number of noncumulative double bonds are inserted, and finally indicated hydrogen is cited, consistent with the structure of the ring system, for all positions that are saturated, i.e., where there are two ring bonds and sufficient ‘exo’ bonds to satisfy the bonding number of the atom.

(b) A fusion name can only be used for preferred IUPAC names when at least two rings of five or more members are present, which is consistent with recommendations in the 1979 edition (ref. 1), but is a change from the recommendations in the 1999 publication on fused ring nomenclature (see FR-0, ref. 4) and the 1993 Guide (ref. 2) where no restriction was placed on the size or number of rings that must be present in order to use the principles of fusion nomenclature. In general nomenclature there is no restriction on the size or number of rings in a fused ring system.

(c) There is no elision of a vowel from fusion prefix names when followed by another vowel in preferred IUPAC names for fused ring systems as prescribed by P-25.3.1.3, which follows Rule R-2.4.1.1 of the 1993 Guide (ref. 2), which abrogated the elision recommended by Rule A-21.4 in the 1979 edition (ref. 1)

(d) Systematic ‘benzo’ names, for example $2H$ -1-benzopyran, are preferred IUPAC names for chromene, isochromene, chromane, isochromane, and their chalcogen analogues used in previous editions (refs. 1, 2, and 4)

(e) A new numbering system is now recommended for ring assemblies consisting of more than two rings or ring systems. The new locant system, composed of composite locants formed from a normal arabic number identifying each ring in order and a superscript number to represent the actual locants of the ring system itself, is recommended for

preferred IUPAC names. The method used in earlier recommendations (refs. 1 and 2), involving serially primed actual locants may be used in general nomenclature.

(f) Unsaturation in ring assemblies is described by ‘ene’, ‘yne’, etc., endings cited after the closing brackets of the ring assembly name; this method allows ring assemblies with unsymmetrically located double bonds to be included in the method. This is a change from the 1979 and the 1993 Guide editions (refs. 1 and 2) and is completely consistent with the method established for spiro compounds in the 1999 publication on nomenclature of spiro compounds (ref. 8).

(g) The ‘a’ prefixes of replacement nomenclature for heterocyclic bridged fused, heterocyclic spiro ring systems, and heterocyclic ring assemblies are cited as nondetachable prefixes and are cited in front of the parent name. This technique allows naming of unsymmetrical heterocycles. Previously, replacement (‘a’) prefixes were cited with the name of the ring to which they belonged.

(h) The following names are now recommended as preselected (see P-12.2) bridge prefixes: ‘sulfano’ for –S–; ‘disulfano’ for –SS–; ‘selano’ for –Se–; ‘tellano’ for –Te–; ‘azano’ for –NH–; epitriazano for –NH-NH-NH–; and –NH-N=N– for epitriaz[1]eno. The bridge prefixes ‘epithio’, ‘epidithio’, ‘episeleno’, ‘epitelluro’, and ‘epimino’ [ref. 4, FR-8.3.1(d)] may be used in general nomenclature.

12. Seniority

(a) Seniority of polycyclic ring systems is now facilitated by a hierarchical order of ring systems, including cyclic and acyclic phane systems. The seniority order of a polycyclic ring system between parent hydrides having the same number of identical heteroatoms, the same number of rings, and the same number of skeletal atoms listed in descending order of seniority as follows: spiro compounds > cyclic phane systems > fusion ring systems > bridged fused ring systems > von Baeyer systems > linear phane systems > ring assemblies. This ordering is a change from earlier recommendations.

(b) In accordance with the seniority of classes (see P-41), compounds such as R-NH-Cl, R-NH-NO, and R-NH-NO₂ are now named as derivatives of amides (see P-67.1.2.6) and compounds such as R-NH-OH are named as *N*-derivatives of the senior amine and not as *N*-derivatives of hydroxylamine, NH₂-OH (see P-62.4, P-68.3.1.1) as in previous recommendations.

13. Adducts

Adducts composed solely of organic compounds have their individual components cited in formulas in the order of seniority of classes (see P-41) no longer according to the number of species in the adduct, nor in accordance with the alphanumerical order as recommended in the 1979 Recommendations (see Rule D-1.55, ref. 1) and in the revised Nomenclature of Inorganic Chemistry, 2005 Recommendations (ref. 12). For adducts composed of organic and inorganic compounds, organic compounds precede inorganic compounds in formulas. Names are formed by citing the names of individual components in the order of the formula. The use of order of seniority of classes, a universal system, as a ranking criterion has been preferred to the language dependent alphanumerical order for preferred IUPAC names and in general nomenclature.

14. Enclosing marks

(a) Names such as cyclohexanecarbonyl and benzenesulfonyl are enclosed in parentheses, even though they are simple prefixes, in order to facilitate name interpretation by avoiding the illusion that two parent hydrides are present. This is a change from the 1993 Guide (ref. 2).

(b) When following the normal nesting order for enclosing marks, two or more enclosing marks of the same level are consecutive because independent enclosing marks accommodating other factors such as stereodescriptors must be inserted into an independent nomenclature fragment. The enclosing mark for the independent nomenclature fragment is jumped to the next level to avoid confusion.

(c) In fused ring names, enclosing parentheses are used following the numerical prefixes ‘bis’, ‘tris’, etc. which indicate multiple occurrences of a parent component. This is a change from the recommendations in the 1998 publication on fusion (ref. 4).

(d) All locants which form part of the name of all heterocyclic components in spiro ring systems and phane systems are placed in brackets as in fused ring systems. In the previous recommendations (ref. 5 and ref. 8) the locants of the first cited component were not enclosed in brackets.

15. Esters

The multiplicative operation is applied to naming organic esters. In doing so, the bi- or polyvalent functional class name is the multiplier and as such must be cited as the last organyl group (alkanediyl, arylene, etc.) as a separate word immediately before the name of the acid component denoted by the anion name derived from the appropriate acid (see P-72.2.2.2) rather than alphabetically along with other monovalent organyl groups, as was done in earlier recommendations.

16. Amides

When an amide is the principal function, it must be named as such. Hence, an *N*-acyl group attached to a nitrogen atom of a heterocyclic system is now named as a pseudoketone (see P-64.3). The method of considering amides as substituents on heterocyclic ring systems, described in the 1993 Recommendations (ref. 2), is retained but only for general nomenclature (see also P-66.1.3).

17. Inorganic parent structures

- (a) For consistency in the names of polynuclear oxoacids, the numerical infix ‘di’ has been uniformly used in naming dinuclear ‘hypo’ acids, for example, hypodiphosphorous acid, rather than hypophosphorous acid.
- (b) Amides and hydrazides of nitric and nitrous acids are now named systematically based on nitric or nitrous amide and/or hydrazide, in accordance with the seniority order of classes rather than as nitro and nitroso amines; the latter names can be used in general nomenclature.
- (c) Since the name ‘disulfurous acid’ is used for HO-SO-SO₂-OH in the *Nomenclature of Inorganic Chemistry* (ref. 12), it cannot be used in the systematic way for HO-SO-O-SO-OH. Accordingly, the preselected name for the latter is ‘1,3-dihydroxy-1λ⁴,3λ⁴-dithioxane-1,3-dione’; and the preselected name for the former is sulfuric sulfurous anhydride.

18. Radicals and ions

- (a) Radicals derived from amines and amides are named using suffixes such as ‘-aminylidene’, ‘-amidylidene’, and ‘carboxamidylidene’. In previous recommendations such radicals were named as derivatives of ‘nitrene’, ‘aminylene’, or ‘λ¹-azane’.
- (b) For choosing the senior parent radical, the senior parent anion, and the senior parent cation, the pertinent criterion is the maximum number of radical, anionic, or cationic centers at the skeletal atom first cited in the seniority order of classes (P-41): N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl > O > S > Se > Te > C. In previous recommendations the order was that for the skeletal replacement (‘a’) prefixes.
- (c) The preferred IUPAC name of an anion formed by the removal of a hydron from the chalcogen atom (O, S, Se, and Te) of a peroxyacid characteristic group is formed by replacing the ‘ic acid’ or ‘ous acid’ ending of the acid name by ‘ate’ or ‘ite’, respectively. In previous recommendations (RC-83.1.6, ref. 3), such anions were named on the basis of an anionic parent hydride.
- (d) The use of compound suffixes ‘aminide’, ‘iminide’ and ‘aminediide’ is a change from previous practice where parent anions H₂N⁻ and HN₂²⁻ were used to express amines and imines having negative charge(s).
- (e) Zwitterionic compounds having the ionic centers in the same parent structure are not considered as neutral compounds to which suffixes can be added. In previous recommendations such zwitterionic compounds were considered neutral and suffixes could be added to them.

19. Isotopically modified compounds

- (a) Isotopically modified atoms or groups that are not identically modified in equivalent positions are expressed separately. This is a change from Section H of the 1979 Recommendations (ref. 1) and Chapter R-8 of the 1993 Guide (ref. 2).
- (b) Isotopically labeled hydrogen atoms in hydrogenated macrocyclic ring systems that are not identically modified are expressed separately. This is a change from previous recommendations.

GLOSSARY

Attached component. A ring or ring system that is fused to a parent component in fusion nomenclature; there are first-order attached components, for example ‘benzo’ in benzo[g]quinoline and ‘furo’ and ‘pyrrolo’ in furo[3,2-*h*]pyrrolo[3,4-*a*]carbazole; second-order attached components, for example ‘cyclopenta’ in cyclopenta[4,5]pyrrolo[2,3-*c*]pyridine and ‘pyrano’ in pyrano[3',2':4,5]cyclohepta[1,2-*d*]oxepine; and so on.

Additive operation. A procedure involving the formal assembly of a structure from its component parts without loss of any atoms or groups, for example calcium chloride, styrene oxide, 1,1'-biphenyl, pentyloxy, decahydronaphthalene, and pyridin-1-ium.

Amplificant. A ring or ring system replacing superatom(s) in the amplification operation of phane nomenclature.

Amplification. An operation in phane nomenclature restoring rings or ring systems from superatoms representing them in a phane skeleton name.

Amplification prefix. Names of the amplificants restored from the superatoms cited as nondetachable prefixes in a phane parent name, for example: benzene and pyridina.

Bridge. In von Baeyer alicyclic ring systems, an unbranched chain of atoms, an atom, or a valence bond connecting two bridgehead atoms; in bridged fused ring systems, a bridge can be an atom or a group of atoms, for example ethano, azano, and epoxireno.

Bridgehead atom. In von Baeyer alicyclic ring systems, any skeletal atom of the ring system that is bonded to three or more skeletal atoms (excluding hydrogen). In bridged fused ring systems, an atom of the fused system to which a bridge is attached.

Carbane nomenclature. Principles, rules, and conventions of substitutive nomenclature applied to the parent hydrides of carbon leading to names such as methanamine and cyclohexanol.

Characteristic group. A single heteroatom, such as --Cl , and $=\text{O}$; a heteroatom bearing one or more hydrogen atoms or other heteroatoms, such as --NH_2 , --OH , $\text{--SO}_3\text{H}$, $\text{--PO}_3\text{H}_2$, and --IO_2 ; or a heteroatomic group attached to or containing a single carbon atom, for example --CHO , --CN , --COOH , and --NCO , attached to a parent hydride.

Complex substituent group. A substituent group consisting of a simple substituent group (the parent substituent group) to which is attached a compound substituent group, for example (chloromethyl)phenyl ($\text{ClCH}_2\text{--C}_6\text{H}_4\text{--}$).

Composite locant. A locant composed of two or more parts. In phane nomenclature composite locants are composed of a primary number identifying each amplificant and a superscript number expressing the locant of the amplificant itself, for example 1^1 and 1^2 . In ring assemblies, composite locants consist of an arabic primary number, identifying each ring system, and an arabic superscript number expressing the numbering of the ring or ring system itself, for example 1^1 and 1^2 .

Compound substituent group. A substituent group consisting of two parts, (1) a simple substituent group (the parent substituent group); and (2) one or more simple substitutive atoms or groups, for example, chloromethyl ($\text{ClCH}_2\text{--}$), hydroxysulfanyl (HO-S--), 2,2-dichloroethyl ($\text{Cl}_2\text{CH-CH}_2\text{--}$).

Concatenated substituent group. A compound or complex substituent group formed only by the additive operation, for example sulfonyloxy (HS-O--) and cyclohexyloxy ($\text{C}_6\text{H}_{11}\text{-O--}$).

Detachable prefix. A substituent prefix cited before the name of a parent structure and, with the exception of hydro/dehydro prefixes, subject to alphabetization, for example amino, methyl, and silyl.

Functional class nomenclature. A system in which the principal characteristic group is expressed as a class term, such as chloride, alcohol, or ketone, written as a separate word or words, following a term derived from a parent hydride, for example methyl iodide and ethyl methyl ketone or substituent group, for example: acetyl chloride.

Functionalized parent hydride. A parent hydride with a characteristic group cited as a suffix, for example cyclopentanecarbonitrile.

Functional parent compound. A structure the name of which expresses or implies the presence of one or more characteristic groups and which has one or more substitutable hydrogen atoms attached to at least one of its skeletal atoms, or in which one of its characteristic groups can form at least one kind of functional modification, for example acetic acid, aniline, and phosphonic acid.

Functional replacement nomenclature. A method by which oxygen atoms of characteristic groups and functional parent compounds are replaced by halogen, chalcogen, and/or nitrogen atoms, for example propane-1-thiol and carbonimidic acid. It is a subset of replacement nomenclature, for which see below.

Fusion atom. An atom of a fused ring system which is common to two or more rings.

Fusion nomenclature. A system for naming bi- and polycyclic systems having two or more rings or ring systems joined together by two adjacent common atoms, for example, benzo[*g*]quinoline and cyclopenta[*a*]naphthalene.

General (IUPAC) nomenclature. The principles, rules, and conventions by which names other than preferred IUPAC names (PINs) are generated, for example acetone, propane-1,3-sultim, and thioacetamide.

Generalized ‘ane’ nomenclature. The principles, rules, and conventions of substitutive nomenclature generally applied to parent hydrides of elements in Groups 13, 14, 16, and 17, for example sulfane, diazane, trisilane, and borane.

Hantzsch-Widman name. A name for a heteromonocyclic ring having three- through ten-ring members formed by the original proposals of Hantzsch and Widman in which a prefix or prefixes denoting the hetero atom(s) in the ring is added to stems denoting the size and degree of saturation of the ring, for example 1,2,4-triazole and 1,2-oxazole.

Heterane nomenclature. The principles, rules, and conventions of substitutive nomenclature applied to parent hydrides for elements of Groups 13, 14, 15, 16, and 17, other than carbon, for example disulfane, triarsane, disilane, and borane.

Heteroamine. A compound having an amino group bonded to a heteroatom, for example piperidin-1-amine.

Heteroimine. A compound having an imino group doubly bonded to a heteroatom, for example methylphosphanimine.

Heteroatom. An atom other than carbon belonging to Groups 13, 14, 15, 16, or 17 in the nomenclature of organic compounds, for example N, Si, and Ge.

Heterol. A compound having a hydroxy group bonded to a heteroatom, for example piperidin-1-ol.

Heterone. A compound having an oxygen atom doubly bonded to a heteroatom, for example methylsilanone.

Interior atom. An atom of a fused ring system that is not a peripheral atom.

Ketone. A compound having an oxygen atom doubly bonded to a carbon atom that is itself linked to two carbon atoms, for example propan-2-one ($\text{CH}_3\text{-CO-CH}_3$).

Multiplicative nomenclature. A system that allows the expression of two or more identical cyclic parent hydrides or heterocyclic parent structures linked by di- or polyvalent substituent groups, for example 1,1'-peroxydibenzene and 4,4'-oxydi(cyclohexane-1-carboxylic acid).

Nondetachable prefix. A structure modifying prefix cited before the name of a parent structure and after alphabetized detachable prefixes and the detachable prefixes hydro and/or dehydro prefixes, for example bicyclo, spiro, aza, and nor.

Parent component. The parent component of a fused ring system is the ring or ring system having the highest seniority according to the seniority order of rings and ring systems, for example oxepine in dibenzo[*c,e*]oxepine.

Parent compound (often used in place of Parent structure; see Parent structure)

Parent hydride. An unbranched acyclic, a cyclic structure, or an acyclic/cyclic structure having a systematic or retained name and to which only hydrogen atoms are attached, for example methane, cyclohexane, styrene, and pyridine.

Parent structure. A parent hydride, for example methane; a functional parent compound, for example phenol; a functionalized parent hydride, for example propan-2-one.

Parent substituent group. A simple substituent group attached to a parent hydride or parent structure in a compound substituent group, for example the ethyl group in $\text{ClCH}_2\text{-CH}_2^-$.

Peripheral atom. Any atom that forms part of the outer perimeter of a fused ring system.

Phane parent skeleton. The skeletal graph before the simplication operation and after the amplification operation in phane nomenclature.

Preferred IUPAC name (PIN). A name preferred among two or more names generated from two or more IUPAC recommendations including the many synonyms that have been coined and used over the years, for example disilylacetic acid and 3-chloropropanoic acid.

Preselected name. A name chosen for a noncarbon (inorganic) structure to be used as the basis for derivation of a preferred IUPAC name in the nomenclature of organic compounds, for example hydrazine and disulfane.

Primary locant. In phane nomenclature, an arabic number designating an atom or an amplificant in a phane parent skeleton. In ring assemblies, primary locants designate the rings or ring systems in the numbering of a structure.

Principal characteristic group. The characteristic group chosen for citation at the end of a name by means of a suffix or a class name, or implied by a trivial name, for example, ethanol and acetic acid.

Pseudoester. A compound having the generic formula $\text{R-E}(\text{=O})_x(\text{OZ})$ and chalcogen analogues where $x = 1$ or 2, and Z is not a carbon atom but an element from the following list: B, Al, In, Ga, Tl, Si, Ge, Sn, Pb, N(cyclic), P, As, Sb, Bi, for example silyl acetate.

Pseudoketone. A cyclic compound having a carbonyl group linked to one or two skeletal heteroatoms or an acyclic compound, other than esters or acid anhydrides, having a carbonyl group linked to one carbon atom and one skeletal heteroatom, except for nitrogen and halogens, or an acyclic compound having a carbonyl group linked to a heteroatom belonging to a ring or ring system, for example piperidin-2-one, 1-silylethan-1-one and 1-(piperidin-1-yl)ethan-1-one

Replacement nomenclature. A system in which one single nonhydrogen atom or a group of atoms is exchanged for another single nonhydrogen atom or group of atoms, for example $6\lambda^5$ -phosphaspiro[4.5]decane and phosphorothioic acid. Skeletal replacement, for which see below, and functional replacement nomenclature, for which see above, are subsets of replacement nomenclature.

Retained name. A traditional or common name used either as the preferred IUPAC name or as an alternative name in general nomenclature, for example acetone and aniline.

Semi-systematic name or semi-trivial name. A name in which only a part is used in a systematic sense, for example methane, but-2-ene, and chalcone.

Simple. A term for a single basic element, a simple substituent group consisting of just one part that describes an atom, or group of atoms as a unit, for example methyl ($-\text{CH}_3$), hydroxy ($-\text{OH}$), nitrilo ($-\text{N} <$), and propan-2-yl [$(\text{CH}_3)_2\text{CH}-$]. In bridged fused names, an atom or group of atoms described as a single unit is a simple bridge, for example epoxy, butano, and phospheno.

Simple substituent group. A substituent group with a name consisting of a single part that describes an atom or group of atoms as a unit, for example methyl ($-\text{CH}_3$), hydroxy ($-\text{OH}$), imino ($=\text{NH}$), and propan-2-yl [$(\text{CH}_3)_2\text{CH}-$].

Simplification. An operation in phane nomenclature leading to a simplified skeleton by condensing a ring or ring system to a single atom called a superatom.

Skeletal replacement ('a') nomenclature. A system in which a heteroatom replaces skeletal atoms of a homogeneous parent hydride, for example 8-thia-2,4,6-trisiladecane and 1,2-dicarba-*closos*-dodecaborane(12). It is a subset of replacement nomenclature for which see above.

Spiro nomenclature. A system for naming polycyclic systems with at least one spiro union based on nomenclature for monospiro bicyclic compounds developed by Adolf von Baeyer, for example spiro[4.5]decane.

Subsidiary parent substituent group. A parent substituent attached to the primary parent substituent group of a complex substituent group attached to a parent hydride or a parent structure, for example in the complex substituent group name (2-chloroethyl)phenyl, ClCH₂-CH₂-C₆H₄-, the ethyl group is a subsidiary parent substituent group and the phenyl group the parent substituent group.

Substituent. An atom or group that takes the place of a substitutable hydrogen atom of a parent hydride or parent structure, for example amino, sulfanyl, and methyl.

Substitutive nomenclature. A system involving the exchange of one or more hydrogen atoms of a parent hydride or parent structure, except for hydrogen atoms of a chalcogen atom, by another atom or group of atoms expressed by a suffix or a prefix denoting the atom or group being introduced, for example 1-methylnaphthalene and pentan-1-ol.

Subtractive operation. A method for describing the removal of an atom, ion, or group implicit in a name. Prefixes, suffixes or endings are used, for example 3-norlabdane, propan-2-yl, and hex-2-ene.

Superatom. Atom in a simplified skeleton of a phane system resulting from the simplification of rings or ring systems.

Systematic name. A name composed entirely of specially coined or selected syllables with or without numerical prefixes and other structural symbols and constructed following the rules of a systematic nomenclature, for example cyclopropanecarbonitrile and 2-chloroethan-1-ol.

Trivial name. A name no part of which is used in a systematic sense, for example xanthophyll.

von Baeyer nomenclature. A system for naming polycyclic systems based on the system for naming bicyclic aliphatic ring systems developed by Adolf von Baeyer and including its extension to polycyclic ring systems, for example bicyclo[3.2.1]octane.