

P-26 Phane nomenclature

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P-26.0 Introduction

Phane Nomenclature is specific to cyclic or acyclic compounds composed of rings or ring systems directly linked to each other or linked by atoms or chains.

Cyclophanes are recognized as a class of compounds (ref. 17). The term originally applied to compounds having two 1,4-phenylene groups held face to face by $-\text{[CH}_2\text{]}_n-$ bridges. It now designates compounds having:

- (a) saturated and/or mancude rings or ring systems, or assemblies of saturated and/or mancude rings or ring systems and;
- (b) atoms and/or saturated or unsaturated chains as alternate components of a large ring.

Phane nomenclature is used to name cyclophanes and has been extended to linear compounds containing a minimum of four rings or ring systems. This section is based on the publication 'Phane nomenclature, Part I. Phane parent names (ref. 5) and contains no modifications to the recommendations therein.

P-26.1 Concepts and terminology

Definitions of terms that will be encountered in the construction of phane names are given below. These terms refer to types of operations, to the components of phane names, and to details of structures involved in the operations.

P-26.1.1 Simplification and amplification

The fundamental operations of phane nomenclature are illustrated in Fig. 1. The operation proceeding from left to right is called simplification; the reverse operation is called amplification, or phane replacement.

The simplification operation illustrates the initial step in the process of constructing a phane name, i.e., nomenclaturally significant segments of a complex cyclic structure are replaced by single atom symbols, called superatoms, thus producing a simplified skeleton that can more easily be named. The phane parent hydride name is then formed from the name of the simplified skeleton and of those of the cyclic components (called amplificants) that were simplified to superatoms. In contrast to other bonds associated with the amplificant, the bonds marked by arrows in Fig. 1 do not disappear in the simplification or amplification operations.

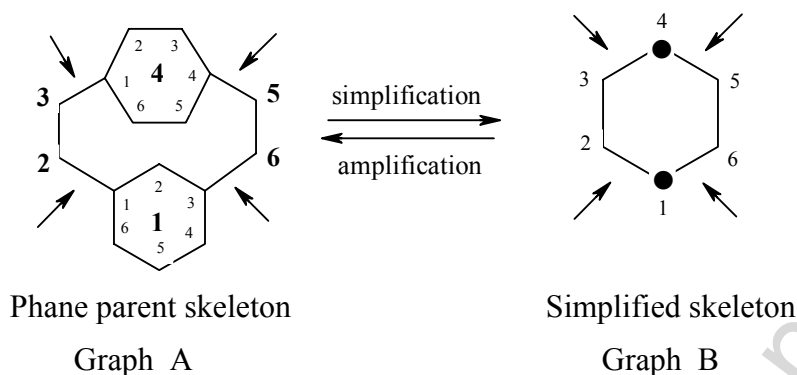


Fig. 1. Phane nomenclature conversion diagram

P-26.1.2 Simplified skeleton of the phane parent hydride, simplified phane parent graph, simplified skeletal name, and skeletal locants.

Graph B in Fig. 1 at which simplification ends and amplification starts is called the simplified skeleton of the phane parent hydride, or simply the simplified skeleton, and is represented by a simplified phane parent graph. Its name is the simplified skeletal name. A simplified skeletal name implies a specific skeletal numbering; its locants are the skeletal locants, which become the primary locants for the phane parent hydride. In Fig. 1, the skeletal locants are denoted by large numbers; they are the same in the simplified skeleton and in the phane parent skeleton.

P-26.1.3 Superatom and superatom locants

The 'atoms' of the simplified skeleton shown by the symbol ● in positions '1' and '4' in Graph B in Fig. 1 that appear on simplification and disappear in amplification are called superatoms. Their locants are called superatom locants.

P-26.1.4 Amplificant, amplification prefix, and amplificant locants.

A multiatomic unit (a ring or a ring system) of structure replacing a superatom in the amplification operation is called an amplificant; the six-membered rings in Graph A are amplificants. They are expressed in a phane parent name by amplification prefixes. Each such prefix implies a specific numbering of the amplificant; the respective locants are called amplificant locants and are shown as the smaller numbers in Graph A.

P-26.1.5 Attachment atoms and attachment locants.

The atoms of an amplificant to which the bonds marked by arrows in Fig. 1 are attached are called attachment atoms and their locants are attachment locants. In Graph A in Fig. 1, amplificant locants '1' and '4' are the attachment locants of the upper ring and amplificant locants '1' and '3' are the attachment locants of the lower ring.

P-26.1.6 Phane parent skeleton, phane parent name, and phane parent hydrides

The skeletal graph at the start of the simplification operation or resulting from an amplification operation is called a phane parent skeleton. Correspondingly, the combination of the simplified skeletal name, amplification prefixes, and the appropriate superatom and attachment locants, is called a phane parent name. The term parent implies that it can be

combined with names for other components derived from the operations of systematic nomenclature of organic chemistry, such as substituent prefixes, hydrogenation prefixes and endings, and characteristic group suffixes. In the absence of such other components, the compound is a phane parent hydride, which means that the name implies the order (valence) of all bonds of the skeletal parent and thus the number of hydrogen atoms attached to each of the skeletal atoms.

P-26.2 Components of phane parent names

P-26.2.1 Simplified skeletal names

P-26.2.2 Amplification prefixes

P-26.2.3 Superatom locants and amplificant attachment locants

P-26.2.1 Simplified skeletal names

A simplified skeletal name consists of the term 'phane' preceded by a prefix denoting the structure of the simplified skeleton; this name is a parent for amplification but for no other operation. The simplification operation must be done in such a way that the amplificants can be expressed by amplification prefixes (see P-26.2.2).

A bond order of one is assumed for all bonds expressed by a simplified skeletal name. Atoms not identified by superatoms represent, by convention, carbon atoms with a bonding number (valence) of four in accordance with the principles of nomenclature of organic compounds.

Superatoms of a simplified skeletal name are assigned the lowest locants or the lowest set of locants, consistent with the numbering of the skeletal class to which it belongs. The lowest set of locants is the one that has the locant with the lowest numerical value at the first point of difference, when the sets are compared term by term in order of increasing value (see P-14.3.4).

Four types of simplified skeletal structures are described below.

P-26.2.1.1 Unbranched acyclic

P-26.2.1.2 Monocyclic

P-26.2.1.3 Polycyclic von Baeyer

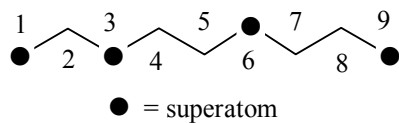
P-26.2.1.4 Spiro

Names of simplified skeletons consists of, in order, of a prefix ('cyclo', 'bicyclo', 'spiro', etc.) indicating the type of structure, a numerical term 'di', 'tri', 'tetra', etc. indicating the number of nodes (including those designating superatoms), and the term phane. No prefix is used to name linearphanes.

The nodes are numbered in accordance with the recommended numbering for each type of structure, as indicated in Chapter 2. Superatoms are given the lowest possible locants.

P-26.2.1.1 Unbranched acyclic skeletal structure

Example:

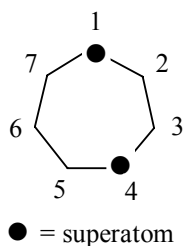


nonaphane

(see first example, P-26.4.1.2 and first example, P-26.5.1)

P-26.2.1.2 Monocyclic skeletal structure

Example:

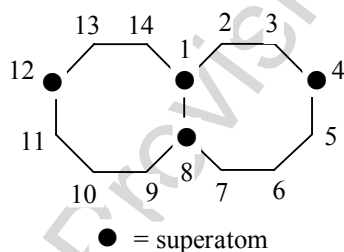


cycloheptaphane

(see first example, P-26.4.1.4; second example, P-26.4.2.2;
and first example, P-26.4.3.3)

P-26.2.1.3 Polyalicyclic (von Baeyer) skeletal structure

Example:

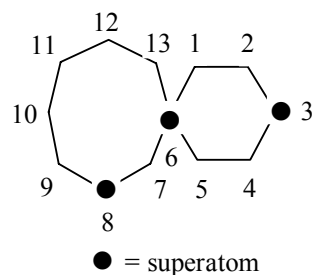


bicyclo[6.6.0]tetradecaphane

(see third example, P-26.4.2.2)

P-26.2.1.4 Spiro skeletal structure

Example:



spiro[5.7]tridecaphane
(see second example, P-26.4.2.4)

P-26.2.2 Amplification prefixes

P-26.2.2.1 Naming amplification prefixes

Names of amplificant prefixes are those of allowed rings or ring systems (see P-26.2.2.2.1) modified by changing the final letter 'e' to 'a', or adding the letter 'a' when no final letter 'e' is present.

Examples:

pyrrole (PIN)	pyrrola (PIN)
furan (PIN)	furana (PIN)
naphthalene (PIN)	naphthalena (PIN)
anthracene (PIN)	anthracena (PIN)

P-26.2.2.2 Parent hydride names for deriving amplification prefixes

P-26.2.2.2.1 Allowed parent hydrides

An amplification prefix can be derived from mancude monocycles and polycycles (having the maximum number of noncumulative double bonds), bridged fused ring systems, saturated monocycles, saturated bicycloalkanes and polycycloalkanes (von Baeyer hydrocarbons), and spiro alkanes. In addition stereoparents are allowed, such as 'gonane' or 'morphinane' (see Chapter 10). Numbering of the parent is retained.

P-26-2.2.2.2 Disallowed names of parent hydrides

(a) the following parent hydride names are not allowed:

- (1) spirobi names such as '1,1'-spirobi[indene] (PIN);
- (2) spiro ring systems with at least one fused ring system or polycycloalkane, such as 'spiro[1,3-dioxolane-2,1'-indene] (PIN) or spiro[bicyclo[2.2.2]octane-2,1'-cyclohexane] (PIN)

- (3) ring assembly names, such as '1,1'-biphenyl' (PIN).
- (b) modified parent hydride names; the corresponding modifications are made once the phane parent hydride has been fully constructed:
- (1) by 'hydro' prefixes, such as '9,10-dihydroanthracene' (PIN);
 - (2) by '-ene' or '-yne' endings, such as 'cyclohexene' (PIN);
 - (3) by 'a' replacement terms, such as '1-azabicyclo[3.2.1]octane' (PIN);
 - (4) by suffixes, such as 'cyclohexanecarboxylic acid' (PIN) and 'cyclohexanone' (PIN);
 - (5) by substitutive prefixes, such as 'ethylbenzene' (PIN).
- (c) functional parent hydrides having retained names, such as 'benzoic acid' (PIN), 'aniline' (PIN).
- (d) names of cyclic compounds formed by functional class nomenclature, such as 'benzyl chloride'.
- (e) partially hydrogenated parent hydride names having retained names, such as 'indane', 'chromane'.

P-26.2.2.3 Order of citation of amplification prefixes

Amplification prefixes are cited in a name in decreasing order of their ring seniority (see P-44.2).

P-26.2.3 Multiple identical amplifiers

Amplifiers occurring more than once in a parent phane skeleton are expressed by use of an appropriate multiplicative term, either 'di', 'tri', etc. or 'bis', 'tris', etc. It is not necessary that the identical amplification prefixes have also identical locants.

P-26.2.3.1 The multiplying prefixes 'di', 'tri', 'tetra', etc. are used in front of simple amplification prefixes, i.e., dibenzena, tripyridina.

P-16.2.4.2 The multiplying prefixes 'bis', 'tris', 'tetrakis', etc. are used before an amplification prefix when it begins with a multiplying prefix as in 'bicyclo[2.2.1]heptane' (PIN), '1,3-dioxole' (PIN); or it begins with a name component that could be preceded by a multiplying prefix indicating a multiple occurrence of that name component, as in '1,4-oxazine' (PIN), '2-benzoxepine' (PIN), or '1,4-methanonaphthalene' (PIN).

P-26.3 Superatom locants and amplifier attachment locants

After the simplified skeletal name and the amplification prefix names have been determined, the phane parent hydride name is completed by adding the locants for the superatoms and the attachment locants. These locants are cited before an amplification prefix; the superatom locant is cited first followed by the attachment locants enclosed in parentheses.

P-26.3.1 Superatom locants

Superatom locants are assigned the lowest locants of the simplified skeleton consistent with the numbering of the class to which it belongs. An amplification prefix preceded by a multiplicative term indicating the presence of like amplifiants requires the appropriate number of superatom locants, which are cited in ascending numerical order.

When like amplifiants also have identical attachment locants, their attachment locants are arranged in ascending numerical order of the first cited superatom locant.

P-26.3.2 Attachment locants

The locants in parentheses in a phane parent hydride name are the attachment locants of the amplifiants whose position in the phane parent skeleton is specified by the preceding superatom locant. The specific order of the attachment locants in the set describes precisely how their respective amplifiants are attached to the rest of the phane parent skeleton. Amplifiants retain the locants of the cyclic parent hydride from which they are derived.

P-26.3.2.1 Identical attachment locant sets for multiple identical amplifiants are cited only once in a name; they follow the set of superatom locants corresponding to the identical amplifiants.

Example:

1,4(1,4)-dibenzencycloheptaphane (PIN)
[not 1(1,4),4(1,4)-dibenzencycloheptaphane;
see second example, P-26.4.1.4]

P-26.3.2.2 The locants in an attachment locant set are arranged so that of any two locants the one cited first is adjacent to the lower locant of the phane parent skeleton.

Example:

1(1,3),4(1,4)-dibenzencycloheptaphane (PIN)
[not 1(1,3)-benzena-4(1,4)-benzencycloheptaphane;
see second example, P-26.4.2.2]

P-26.4 Numbering of phane parent hydrides

The following rules are used for numbering phane parent hydrides. These rules are hierarchical, i.e., each particular rule is applied only to alternatives not eliminated by preceding rules.

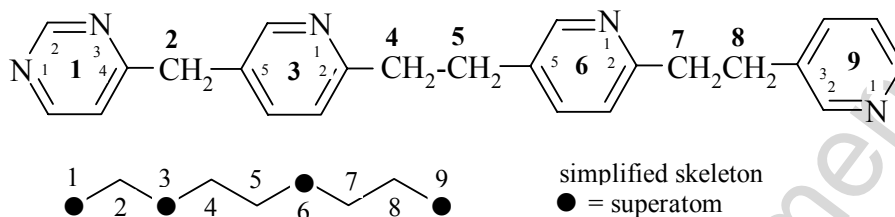
P-26.4.1 Numbering of phane parent skeletons and amplifiants

P-26.4.1.1 The numbering of a phane parent skeleton is first determined by the rules governing the appropriate skeletal class to which it belongs. When because of skeletal symmetry, these rules leave alternatives, the numbering that gives the lowest set of locants for the superatoms is selected. The lowest set of locants is the one that has the lowest numerical value at the first point of difference, when the sets are compared term by term in increasing numerical value, as defined in the general rule P-14.3.4.

P-26.4.1.2 Numbering of an amplificant is determined primarily by the numbering rules that apply to the parent name from which the amplification prefix is derived. When there is a choice, the general rule of lowest locants is used, as described in the preceding rule.

These two rules, P-26.4.1.1 and P-26.4.1.2, are exemplified by the following examples.

Examples:



1(4)-pyrimidina-3,6(5,2),9(3)-tripyridinanonaphane (PIN)

[not 9(4)-pyrimidina-1(3),4,7(2,5)-tripyridinanonaphane]

[see P-26.2.1.1 and P-26.4.1.1; the superatom locant set of the correct name, '1,3,6,9', is lower than '1,4,7,9']

[not 1(4)-pyrimidina-3,6(2,5),9(3)-tripyridinanonaphane]

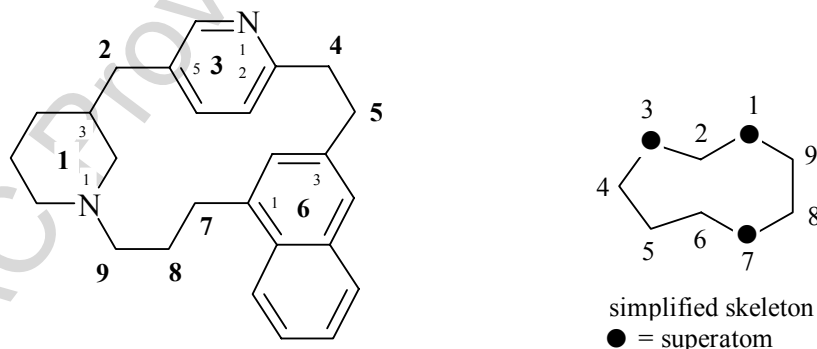
[see P-26.3.2.2; the first locant of the attachment locant set '(2,5)' is not the locant adjacent to the lower locant of the simplified skeleton]

[not 1(4)-pyrimidina-3(5,2),6(5,2),9(3)-tripyridinanonaphane]

[see P-26.3.2.1; the identical attachment locant sets '(5,2)' must be contracted to '3,6(5,2)']

[not 1(4)-pyrimidina-3,6(3,6),9(3)-tripyridinanonaphane]

[see P-26.4.1.2; the attachment locant set '(5,2)' of the pyridine amplificant in the correct name, written in the ascending numerical order '(2,5)' for comparison, is lower than the set '(3,6)']



3(5,2)-pyridina-1(3,1)-piperidina-6(3,1)-naphthalenacyclononaphane (PIN)

[not 1(5,2)-pyridina-3(3,1)-piperidina-7(3,1)-naphthalenacyclononaphane]

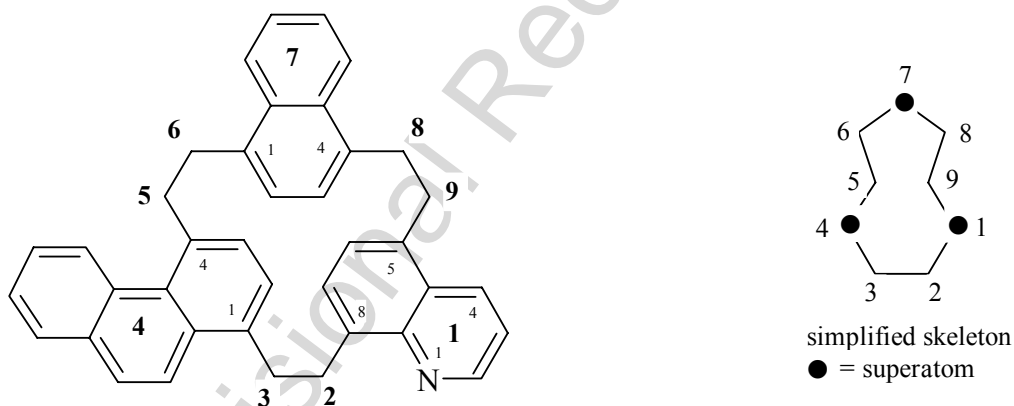
[not 7(5,2)-pyridina-5(1,3)-piperidina-1(3,1)-naphthalenacyclononaphane]

[see P-26.4.2.1; the superatom locant set of the correct name '1,3,6' is lower than the locant set '1,5,7' in either of the above names]

[not 3(2,5)-pyridina-1(1,3)-piperidina-6(1,3)-naphthalenacyclononaphane]
[see P-26.3.2.2; the first locant of each the attachment locant sets '(2,5)', '(1,3)' and '(1,3)' for the pyridine, piperidine, and naphthalene amplificants, respectively, is not the locant adjacent to the lower locant of the parent phane skeleton]

P-26.4.1.3 Amplification of symmetrical simplified phane skeletons with at least two superatoms representing different amplificants results in the loss of symmetry and creates numbering alternatives. In such cases, the lower available superatom locant is assigned to an amplificant that appears earlier in the seniority of rings and ring systems (see P-44.2). The application of this procedure may require a sequence of steps. First, the lowest available superatom locant(s) is (are) assigned to the amplificants appearing first in the seniority order. Then, the same procedure is applied successively to assign remaining superatom locants to the rest of the amplificants.

Example:



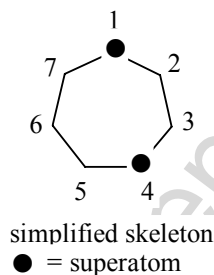
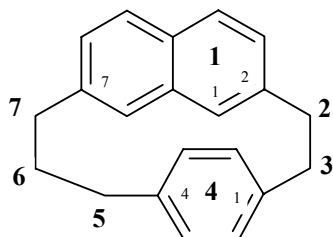
1(8,5)-quinolona-4(1,4)-phenanthrena-7(1,4)-naphthalenacyclononaphane (PIN)

[not 1(8,5)-quinolona-4(1,4)-naphthalena-7(4,1)-phenanthrenacyclononaphane]
[the senior amplificant is quinoline (see P-44.2) and must receive the lowest superatom locant '1'; the phenanthrene amplificant is second in seniority (see P-44.2) and therefore must be given the second lowest superatom locant, '4']

[not 1(8,5)-quinolona-4(4,1)-phenanthrena-7(1,4)-naphthalenacyclononaphane]
[see P-26.3.2.2; the attachment locants of phenanthrene amplificant, '(4,1)' are not correctly cited; the first locant of the attachment locant set is not the locant adjacent to the lower locant of the phane parent skeleton, '3']

P-26.4.1.4 When, because of symmetry, these rules leave a choice, an amplificant is numbered in such a way that the lower attachment locant is adjacent to the lower locant of the phane parent skeleton.

Examples:



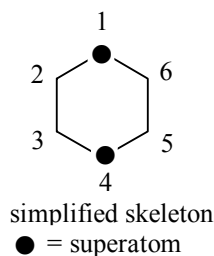
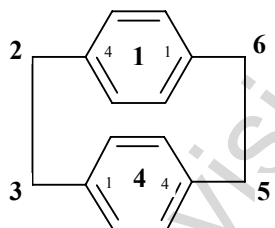
1(2,7)-naphthalena-4(1,4)-benzenacycloheptaphane (PIN)

[see P-26.4.1.2 and P-26 4.1.1; the lowest locant set for the superatoms in the phane parent skeleton is '1,4'; the senior amplificant, naphthalene (see P-44.2), must be assigned to the superatom locant '1']

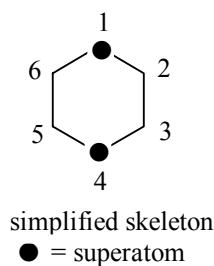
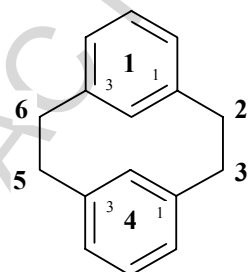
[not 1(2,7)-naphthalena-4(4,1)-benzenacycloheptaphane]

[not 1(7,2)-naphthalena-4(4,1)-benzenacycloheptaphane]

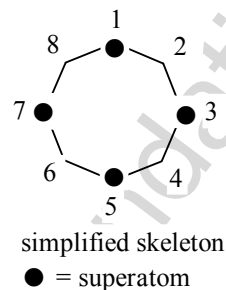
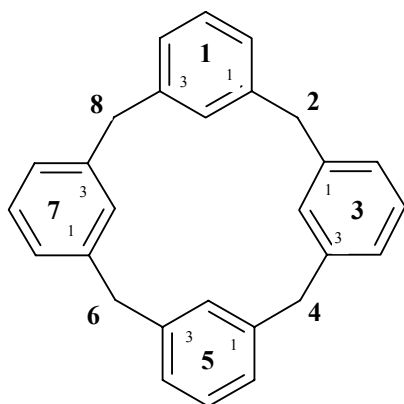
[the correct citation for the attachment locant sets, '(1,4)' for benzene and '(2,7)' for naphthalene, places the lower attachment locant adjacent to the lower locant of the phane skeleton]



1,4(1,4)-dibenzenacyclohexaphane (PIN)



1,4(1,3)-dibenzenacyclohexaphane (PIN)



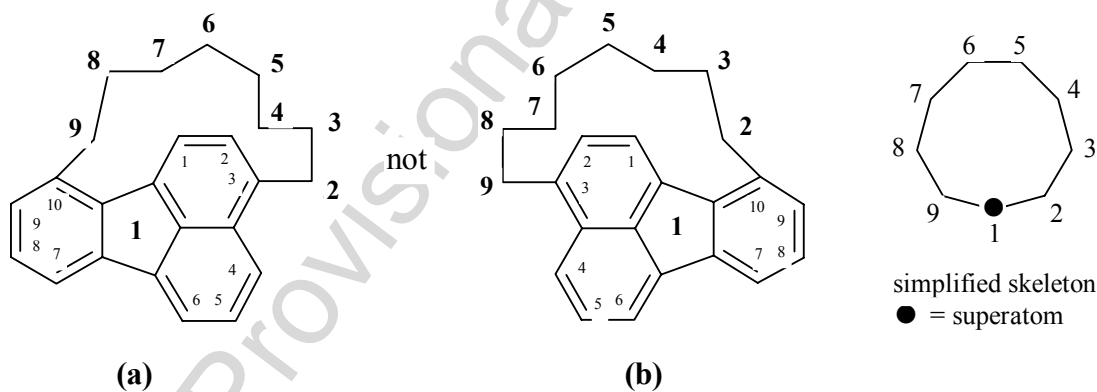
1,3,5,7(1,3)-tetrabenzenacyclooctaphane (PIN)

P-26.4.2 Numbering of simplified phane skeletons with respect to amplificant numbering

Numbering alternatives are found in symmetrical simplified skeletons when amplification by a single unsymmetrical amplificant or by identical amplifiants having different attachment locants removes the symmetry. Choice among such alternatives is made according to the following rules.

P-26.4.2.1 When a single amplificant is unsymmetrical, the lower locant of the phane parent skeleton must be adjacent to the lower attachment locant of the amplificant.

Example:



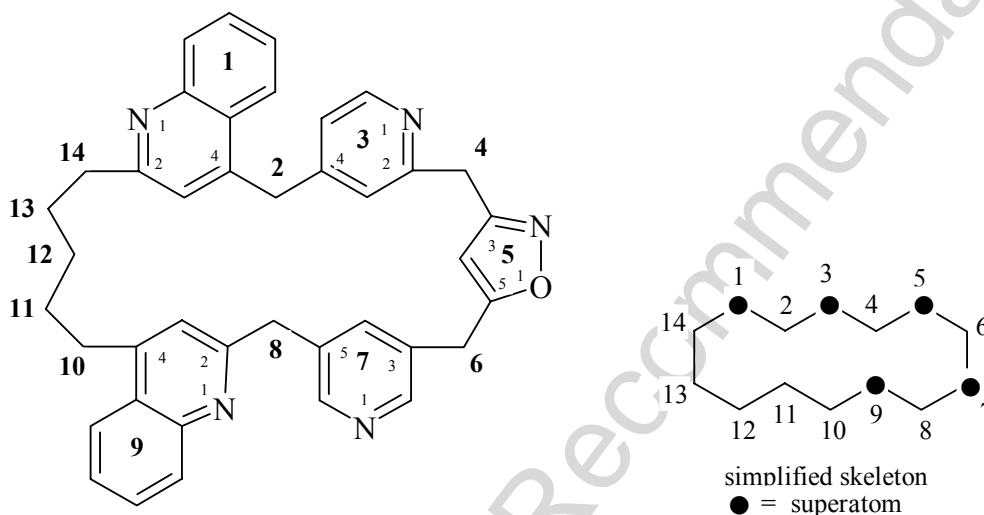
1(3,10)-fluoranthenacyclononaphane (a) (PIN)

[not 1(10,3)-fluoranthenacyclononaphane (b)]

(the lower amplificant locant '3' must be adjacent to the lower skeletal locant '2')

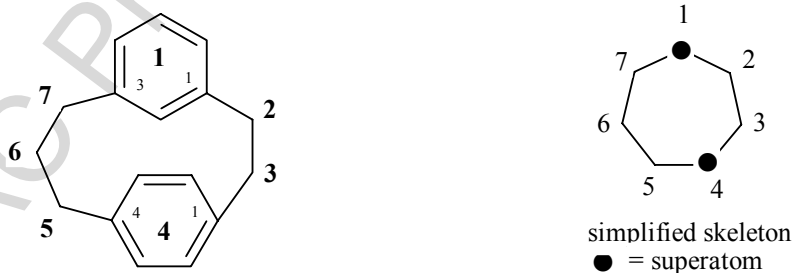
P-26.4.2.2 When two amplificants can be given the lower of two superatom locants, the lower locant is assigned to the superatom representing the amplificant with the lower set of attachment locants. When necessary, this procedure is applied to other amplificants in accordance with their order of seniority until two or more identical amplificants have different attachment locants (see last example).

Examples:



1(4,2),9(2,4)-diquinolina-3(4,2),7(3,5)-dipyridina-5(3,5)-[1,2]oxazolacyclotetradecaphane (PIN)

[not 1,9(2,4)-diquinolina-3(5,3),7(2,4)-dipyridina-5(3,5)-[1,2]oxazolacyclotetradecaphane]
 [the attachment locant set for the senior quinoline amplificants (see P-26.2.2.3), '4,2' and '2,4', respectively, when compared in ascending numerical order are the same, but when the attachment locant sets for the pyridine amplificants, '(4,2)' and '(5,3)', respectively, are compared in ascending numerical order, '(2,4)' and '(3,5)', respectively, the former is lower and therefore the attachment locant set '(4,2)' is associated with the superatom with the lower locant '3']



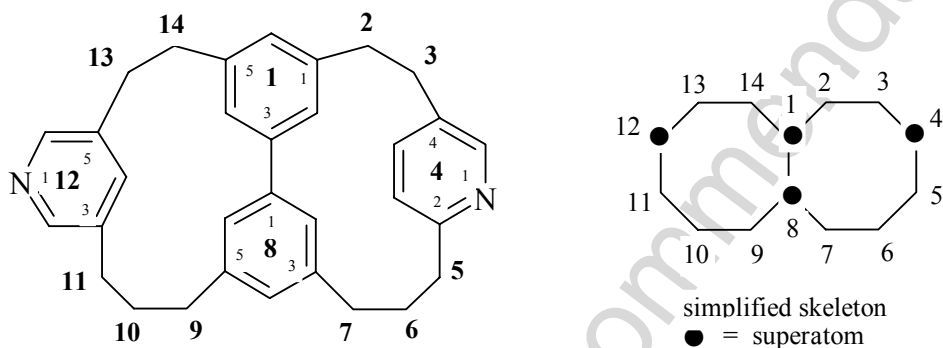
1(1,3),4(1,4)-dibenzenacycloheptaphane (PIN)

[not 1(1,4),4(1,3)-dibenzenacycloheptaphane]

(the lower attachment locant set '(1,3)' is not associated with the superatom having the lower locant)

[not 1(1,3),4(4,1)-dibenzenacycloheptaphane]

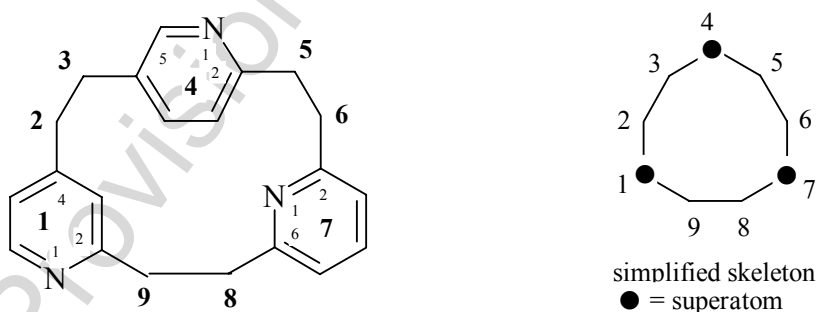
(in the attachment locant set (4,1), the first locant is not the one adjacent to the lower locant of the phane parent skeleton, see P-26.3.2.2)



4(5,2),12(3,5)-dipyridina-1,8(1,3,5)-dibenzenabicyclo[6.6.0]tetradecaphane (PIN)

[not 4(3,5),12(2,5)-dipyridina-1,8(1,3,5)-dibenzenabicyclo[6.6.0]tetradecaphane]

[for the pyridine amplificant the attachment locant set '(5,2)', when compared in ascending numerical order, i.e., '(2,5)', is lower than '(3,5)'; therefore the pyridine amplificant with the locant set '(5,2)' must be associated with the lower superatom locant, '4']



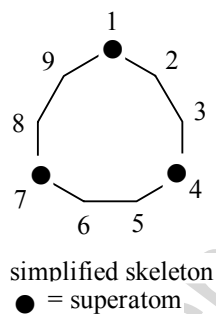
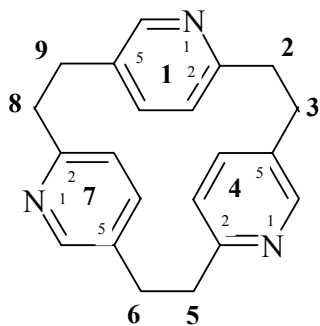
1(4,2), 4(5,2), 7(2,6)-tripyridinacyclononaphane (PIN)

[the attachment locant sets '(2,4)', '(2,5)' and '(2,6)' must be assigned to superatoms '1', '4', and '7', respectively; the arrangement of the locants in each set is governed by P-26.3.2.2]

P-26.4.2.3 If, after the application of P-26.4.2.2, a choice is still necessary and a single unsymmetrical amplificant remains, P-26.4.2.1 is applied to the single unsymmetrical amplificant.

Example:

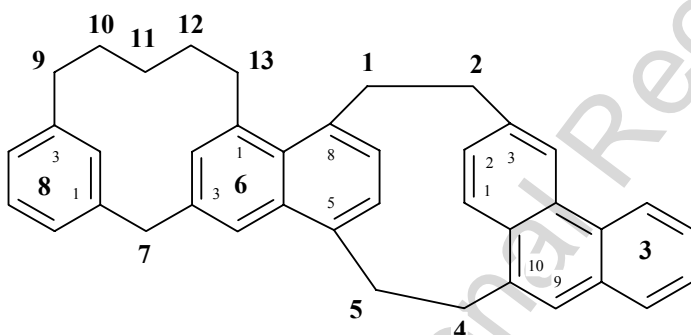
Examples:



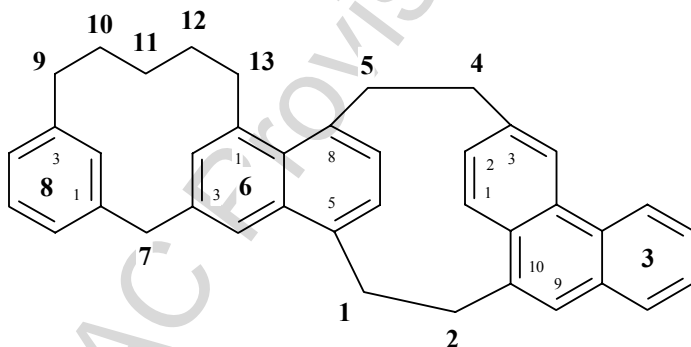
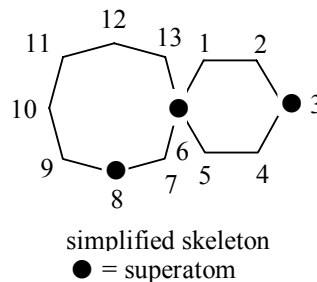
1(2,5),4,7(5,2)-tripyridinacyclononaphane (PIN)

[not 1(5,2),4,7(2,5)-tripyridinacyclononaphane]

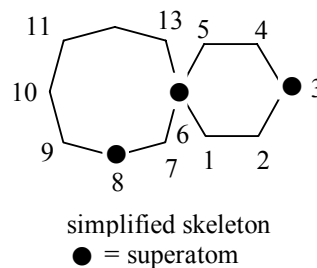
[when compared in the order of increasing value of the corresponding superatoms, the amplificant locant set '(2,5)(5,2)(5,2)' in the correct name is lower than '(5,2)(2,5)(2,5)']



I
 not



II



3(3,10)-phenanthrena-6(8,5,3,1)-naphthalena-8(1,3)-benzenaspiro[5.7]tridecaphane (PIN)

[not 3(10,3)-phenanthrena-6(5,8,3,1)-naphthalena-8(1,3)-benzenaspiro[5.7]tridecane]

[the set of attachment locants '(3,10)(8,5,3,1)(1,3)' in the correct name cited for comparison in the in order of the increasing value of their corresponding superatom

locants, is lower than '(10,3)(5,8,3,1)(1,3)', the corresponding set of attachment in the incorrect name]

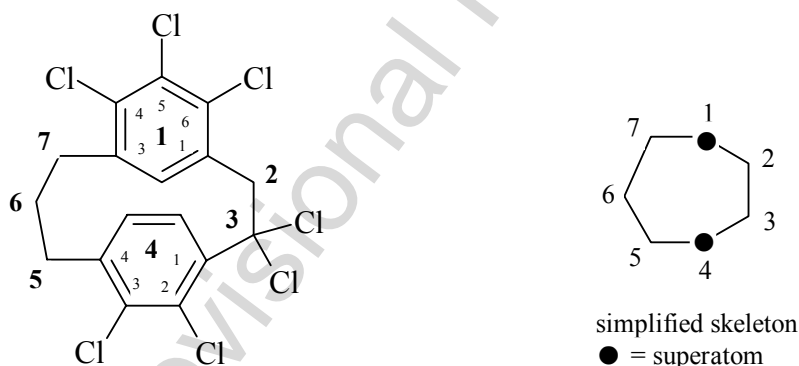
P-26.4.3 Numbering of phane parent hydrides

P-26.4.3.1 In a phane parent hydride, the locants for atoms that do not belong to amplificants are the locants of the simplified skeleton. However, locants for the atoms of the amplificants must be distinguished from the arabic number locants of the simplified skeleton. Thus, locants for amplificant atoms are constructed by citing the actual locants of the amplificant as superscripts to the locant of the superatom that represents the amplificant in the simplified skeleton.

P-26.4.3.2 In a substituted phane parent hydride name, a series of composite locants based on the superatom locant must not be contracted. As it is the rule for citing locants in front of detachable prefixes, there must be a number of locants corresponding to the multiplying prefix, 'di', 'tri', etc. in front of the prefix.

P-26.4.3.3 The seniority of a composite locant is determined first on the basis of its primary locants, i.e., the locants of the phane parent skeleton, and, if these locants are identical, on the basis of the complete composite locant itself, i.e., the primary locant and its superscripts.

Examples:



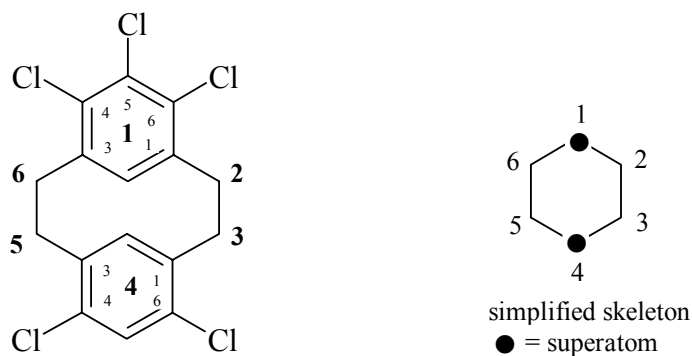
$1^4, 1^5, 1^6, 3, 3, 4^2, 4^3$ -heptachloro-1(1,3),4(1,4)-dibenzocycloheptaphane (PIN)

[not $1^{4,5,6}, 3, 3, 4^{2,3}$ -heptachloro-1(1,3),4(1,4)-dibenzocycloheptaphane]

[superscript locants denoting positions on amplificants are not contracted
 (see P-26.4.3.2)]

[not $1^2, 1^3, 2, 2, 4^4, 4^5, 4^6$ -heptachloro-1(1,4),4(1,3)-dibenzocycloheptaphane]

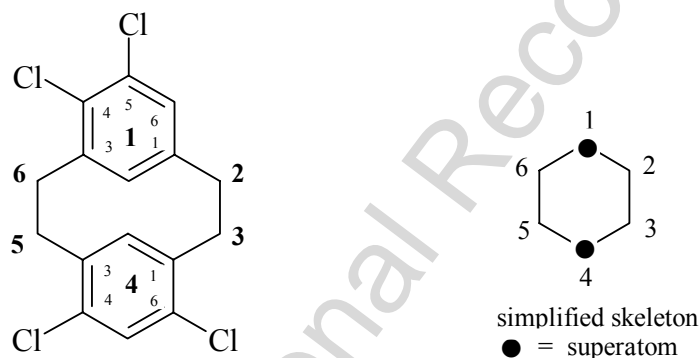
[the amplificant with the lower attachment locant set is not assigned to the superatom with the lowest locant (see P-26.4.3.3)]



$1^4, 1^5, 1^6, 4^4, 4^6$ -pentachloro-1,4(1,3)-dibenzencyclohexaphane (PIN)

[not $1^4, 1^6, 4^4, 4^5, 4^6$ -pentachloro-1,4(1,3)-dibenzencyclohexaphane]

[the primary locant set '1,1,1,4,4' is lower than the locant set '1,1,4,4,4'
 (see P-26.4.3.3)]



$1^4, 1^5, 4^4, 4^6$ -tetrachloro-1,4(1,3)-dibenzencyclohexaphane (PIN)

[not $1^4, 1^6, 4^5, 4^6$ -tetrachloro-1,4(1,3)-dibenzencyclohexaphane]

[the primary locant sets '1,1,4,4' are identical but the composite locant set ' $1^4, 1^5, 4^4, 4^6$ ' is lower than ' $1^4, 1^6, 4^5, 4^6$ ' (see P-26.4.3.3)]

P-26.5 Skeletal replacement ('a') nomenclature in phane nomenclature

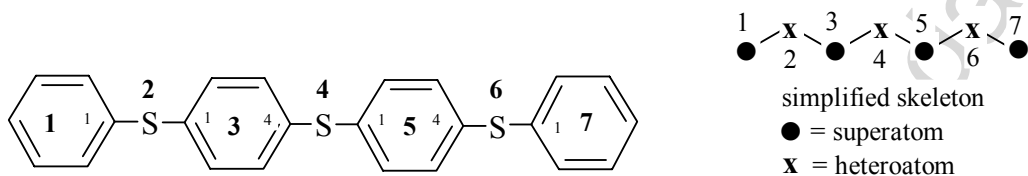
Skeletal replacement ('a') nomenclature is applied in two ways in phane nomenclature:

- (1) to name phane parent hydrides having heteroatoms located in the simplified parent skeleton, i.e., heteroatoms not in names of amplification prefixes;
- (2) to indicate heteroatoms in heterocyclic amplifiants whose names cannot be used as amplification prefixes because they, themselves, are named by skeletal replacement ('a') nomenclature, for example, heteromonocycles having more than ten members and polycyclic von Baeyer systems.

The general principles, conventions and rules described for skeletal replacement ('a') nomenclature in Section P-15.4 are fully applicable to the appropriate phane parent hydrides.

P-26.5.1 Skeletal replacement ('a') nomenclature in simplified plane names is accomplished in two steps. First, the parent plane hydrocarbon is named and then the heteroatoms are denoted by means of nondetachable 'a' prefixes cited in front of the name so created. Locants for the heteroatoms are assigned according to the numbering of the simplified parent skeleton.

Examples:



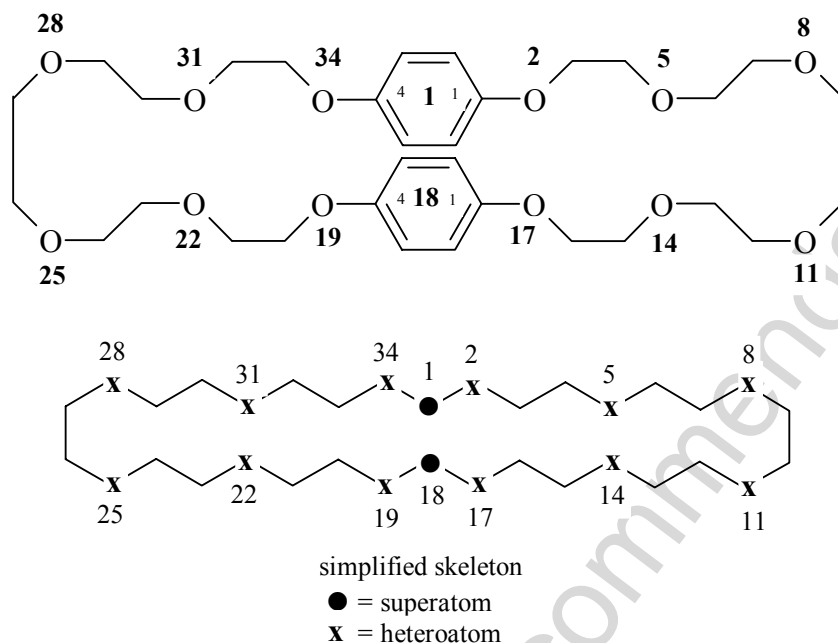
Step 1: 1,7(1),3,5(1,4)-tetrabenzenaheptaphane

Step 2: 2,4,6-trithia-1,9(1),3,5(1,4)-tetrabenzenaheptaphane (PIN)



Step 1: 1(3,5)-[1,2]oxazola-5(1,4)-cyclohexanacyclooctaphane

Step 2: 3,7-dithia-1(3,5)-[1,2]oxazola-5(1,4)-cyclohexanacyclooctaphane (PIN)



Step 1: 1,18(1,4)-dibenzenacyclotettratriacontaphane

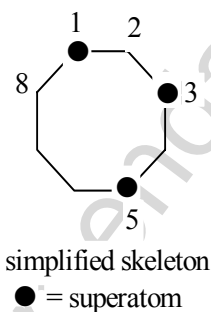
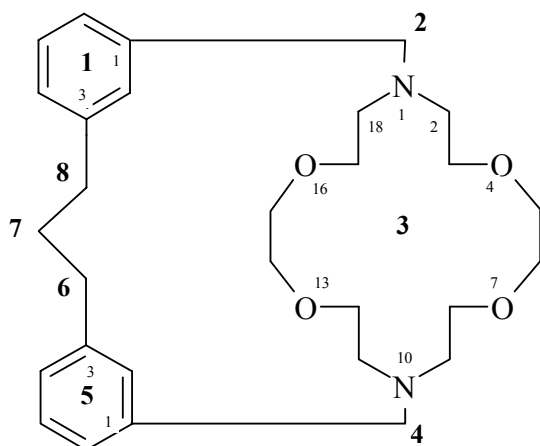
Step 2: 2,5,8,11,14,17,19,22,25,28,31,34-dodecaoxa-1,18(1,4)-
dibenzenacyclotettratriacontaphane (PIN)

P-26.5.2 Skeletal replacement ('a') nomenclature in amplificants

Locants for heteroatoms in amplificants are assigned according to the numbering of the simplified skeleton and the position of heteroatoms in the amplificants following the instructions in P-26.4 for substituent locants. Thus, positions of heteroatoms in amplificants are described by composite locants.

Note: Since the numbering of the heteroamplificant is fixed by the locants of the corresponding hydrocarbon amplificant, the numbering of the heteroatoms may not correspond to the numbering of the heteromonocycle, itself.

Example:



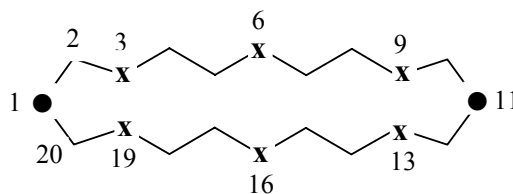
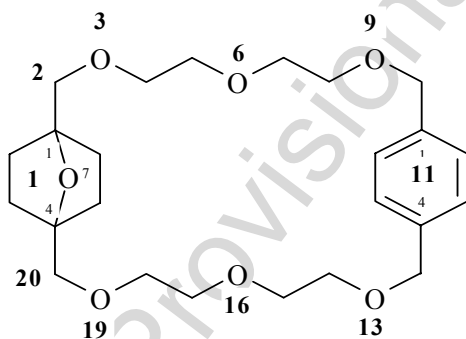
Step 1: 3(1,10)-cyclooctadecana-1,5(1,3)-dibenzenacyclooctaphane

Step 2: 3<sup>4,3<sup>7,3<sup>13,3¹⁶-tetraoxa-3<sup>1,3¹⁰-dianza-3(1,10)-cyclooctadecana-1,5(1,3)-
 dibenzenacyclooctaphane (PIN)</sup></sup></sup></sup>

P-26.5.3 Simultaneous skeletal replacement ('a') in simplified skeletal names and amplificants

When skeletal replacement occurs in both simplified skeletons and in amplificants both P-26.5.1 and P-26.5.2 are applied.

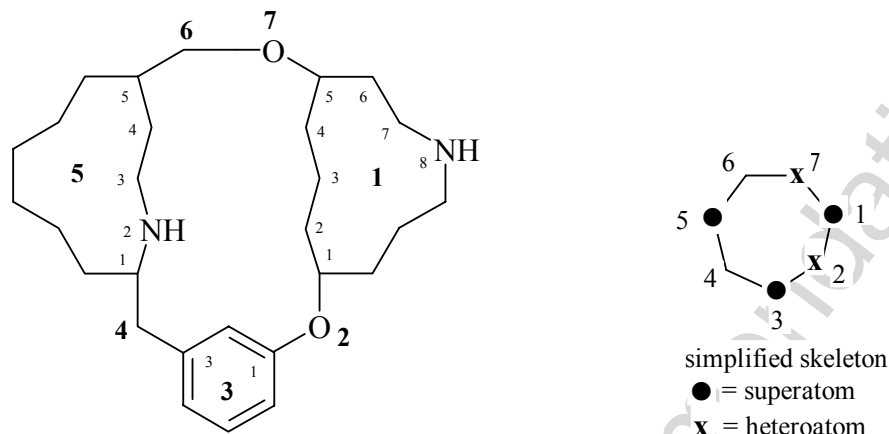
Example:



simplified skeleton
 ● = superatom
 X = heteroatom

Step 1: 1(1,4)-bicyclo[2.2.1]heptana-11(1,4)-benzenacycloicosaphane

Step 2: 1^{7,3,6,9,13,16,19}-heptaoxa-1(1,4)-bicyclo[2.2.1]heptana-11(1,4)-
 benzenacycloicosaphane (PIN)



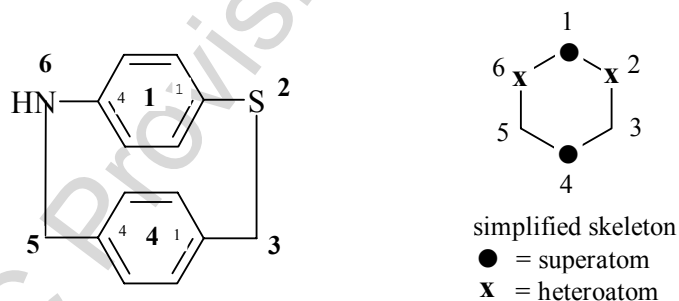
Step 1: 1,5(1,5)-dicycloundecana-3(1,3)-benzenacycloheptaphane

Step 2: 2,7-dioxa-1⁸,5²-diaz-1,5(1,5)-dicycloundecana-3(1,3)-benzenacycloheptaphane (PIN)

[not 4,6-dioxa-1²,5⁸-diaz-1,5(1,5)-dicycloundecana-3(1,3)-benzenacycloheptaphane]
 [the primary locant set for the heteroatoms in the correct name, cited for comparison in ascending order '1,2,5,7', is lower than the locant set '1,4,5,6']

P-26.5.4.2 Lowest locants are assigned to heteroatoms considered in the order of their seniority: O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl (see P-15.4), first with regard to the set for primary locants for heteroatoms, i.e., the locants of the simplified skeleton (the locants without including any superscript numbers), and then, if these locants are identical, to the set of the complete heteroatom locants, which includes the primary locants and the superscript numbers (see P-26.4.3.3).

Examples:

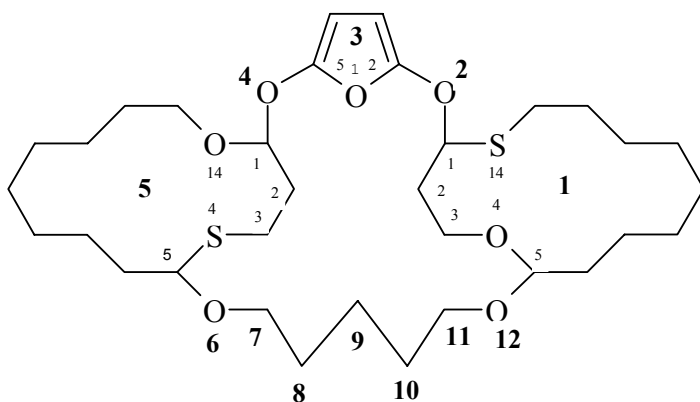


Step 1: 1,4(1,4)-dibenzenacyclohexaphane

Step 2: 2-thia-6-aza-1,4(1,4)-dibenzenacyclohexaphane (PIN)

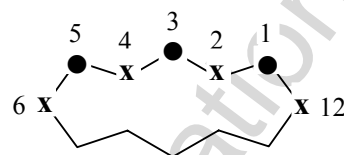
[not 6-thia-2-aza-1,4(1,4)-dibenzenacyclohexaphane]

[since the 'a' prefix 'thia' is senior to 'aza' in skeletal replacement ('a') nomenclature (see P-15.4), it must be given the lower locant]



I

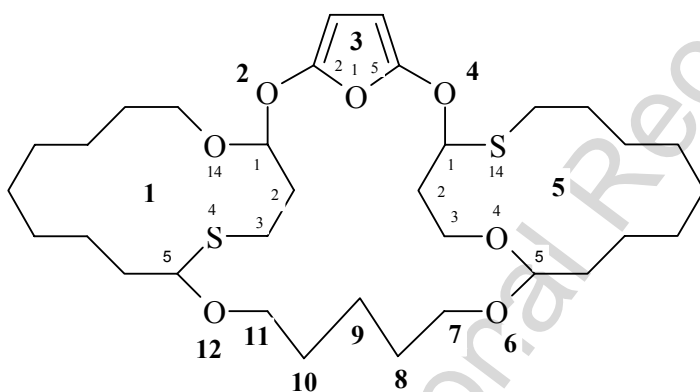
not



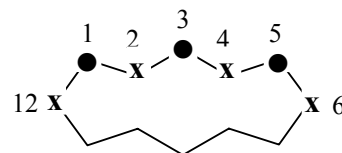
simplified skeleton

● = superatom

X = heteroatom



II



simplified skeleton

● = superatom

X = heteroatom

Step 1: 3(2,5)-furana-1,5(1,5)-dicyclotetradecanacyclododecaphane

Step 2: 1⁴,2,4,5¹⁴,6,12-hexaoxa-1¹⁴,5⁴-dithia-3(2,5)-furana-1,5(1,5)dicyclotetradecanacyclododecaphane (**I**) (PIN)

[not 1¹⁴,2,4,5⁴,6,12-hexaoxa-1⁴,5¹⁴-dithia-3(2,5)-furana-1,5(1,5)-dicyclotetradecanacyclododecaphane (**II**)]

[application of P-26.5.4.1 reveals that both the primary locant sets and the primary locant sets including the composite locants for the heteroatoms without regard to the kind of heteroatom are the same for both names, '1,1,2,4,5,5,6,12' and '1⁴,1¹⁴,2,4,5⁴,5¹⁴,6,12', respectively. The primary locant sets for the senior prefix 'oxa'

are also the same in both cases, '1,2,4,5,6,12', but for the locant sets including composite locants, the locant set for the prefix 'oxa' in the correct name, 1⁴,2,4,5¹⁴,6,12, is lower than the locant set for 'oxa' in the incorrect name, '1¹⁴,2,4,5⁴,6,12']

P-27 Fullerenes

P-27-0 Introduction

A preliminary survey of the nomenclature and terminology of fullerenes was published in 1997 (ref. 19). This Section is based on the IUPAC Recommendations 2002 (ref. 10), that deal in depth with two fullerenes, i.e. the most commonly known fullerene having 60 carbon atoms and one of its C-70 homologues.

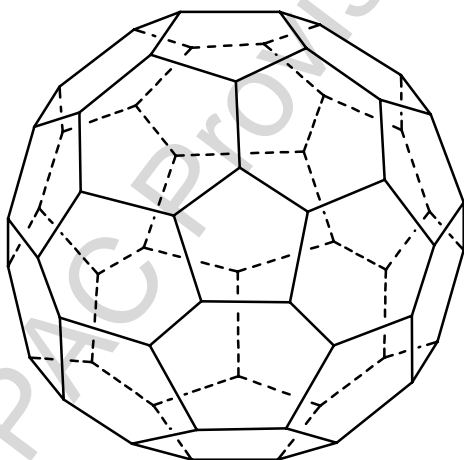
This Section is devoted to parent hydrides only. Derivatives are described in Chapter 6, radicals and ions are discussed in Chapter 7. Chapter 8 includes a brief mention of fullerenes in the discussion on the configurational notation.

- P-27.1 Definitions
- P-27.2 Fullerene names
- P-27.3 Numbering of fullerenes
- P-27.4 Structurally modified fullerenes
- P-27.5 Replacement of skeletal atoms
- P-27.6 Addition of rings and ring systems

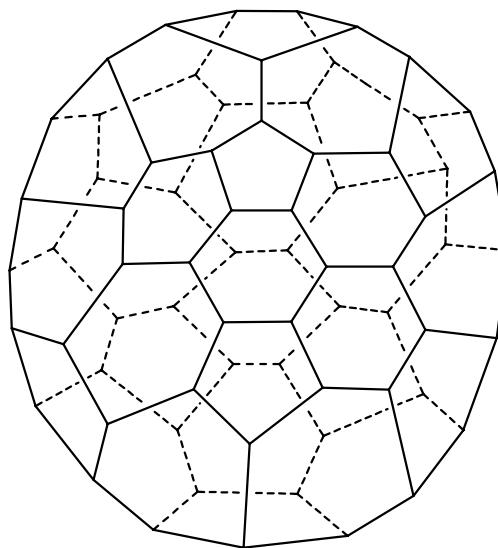
P-27.1 Definitions

P-27.1.1 Fullerenes

Fullerenes are compounds composed solely of an even number of carbon atoms, which form a cage-like fused ring polycyclic system with twelve five-membered rings and the rest six-membered rings (see ref. 17). The archetypal example is [60]fullerene, where the atoms and bonds delineate a truncated icosahedron. The term has been broadened to include any closed cage structure consisting entirely of three-coordinate carbon atoms.



(C₆₀-I_h)[5,6]fullerene



(C₇₀-D_{5h(6)})[5,6]fullerene

P-27.1.2 Fullerenes

Fullerenes are fully saturated fullerenes, for example, $C_{60}H_{60}$.

P-27.1.3 Fulleroids

Heterofullerenes, norfullerenes, homofullerenes, and secofullerenes have been called 'fulleroids' (fullerene-like), because they resemble fullerenes in structure but do not conform to the definition of a fullerene as given above. It is convenient to refer to them as fulleroids and name them as modified fullerenes.

P-27.2 Fullerene names

P-27.2.1 Systematic names

The recommended systematic names for fullerenes include the number of carbon atoms, the point group symbol, the size of the rings, the relative arrangement of rings, and the term 'fullerene', all combined to give names, such as $(C_{60}-I_h)[5,6]$ fullerene and $(C_{70}-D_{5h(6)})[5,6]$ fullerene for the two fullerenes discussed in this Section. The parenthetical prefix gives the carbon content and the point group symbol and the bracketed numbers indicate the ring sizes in the fullerene. The latter is important in fullerenes with rings other than five- and six-membered. The subscript (6) following the point group symbol D_{5h} in the latter name indicates that the five-membered ring on the five-fold symmetry axis is surrounded by six-membered rings. This differentiates this fullerene from an isomeric fullerene which has five-membered rings surrounding the five-membered ring on the five fold symmetry axis, which would have the name $(C_{70}-D_{5h(5)})[5,6]$ fullerene.

The recommended names have the same information as the corresponding names used by the Chemical Abstracts Service (CAS), but in a different format. The corresponding CAS names are [5,6]fullerene- $C_{60}-I_h$ and [5,6]fullerene- $C_{70}-D_{5h(6)}$, respectively (see ref. 10).

P-27.2.2 Trivial names

The names [60- I_h]fullerene and [70- D_{5h}]fullerene (shortened to [60]fullerene and [70- D_{5h}]fullerene in usage) given in the IUPAC Preliminary Survey (ref. 19) are names first introduced in the literature for the $(C_{60}-I_h)[5,6]$ and $(C_{70}-D_{5h(6)})[5,6]$ fullerenes. They were based on the limited definition of fullerenes restricted to five and six-membered rings. Since important information is missing from these names, they are considered as trivial names only for these specific compounds.

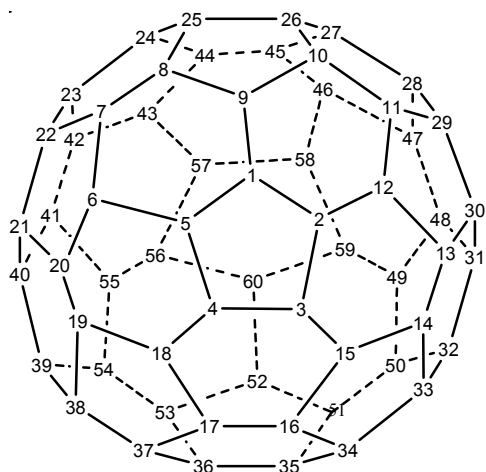
P-27.2.3 Preferred IUPAC names

IUPAC systematic names are preferred to CAS and trivial names. These names are not fully interchangeable. They each depend on a specific methodology for generating names of derivatives. But, most important, they do correspond to different numbering systems, one for IUPAC systematic and CAS names, another one for trivial names (see P-27.3). Preferred names for fullerenes and fullerene derivatives are those that use preferred components when a choice is possible.

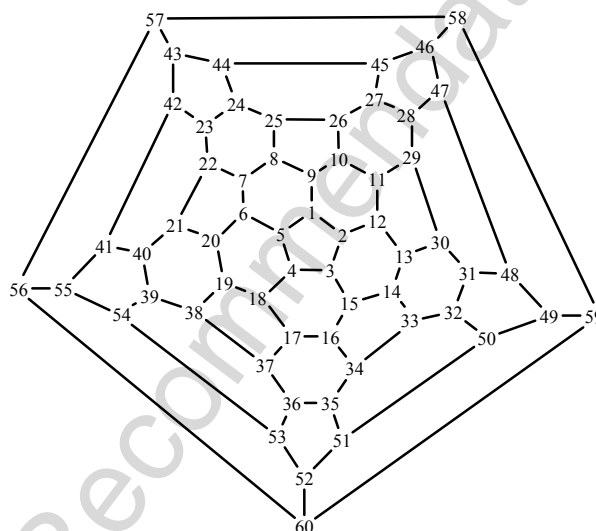
P-27.3 Numbering of fullerenes

Systematic numbering is not yet a fully solved issue in the nomenclature of fullerenes. The objectives are to achieve a continuous numbering and use a well defined starting point for all fullerenes. Studies are still underway. The criteria for numbering the $(C_{60}-I_h)[5,6]$ fullerene and $(C_{70}-D_{5h(6)})[5,6]$ fullerene are discussed in the IUPAC publication (ref. 10). It is important to note that the

systematic numbering used with IUPAC systematic names is derived from the system developed by the Chemical Abstracts Service and that the two systems are identical for these two specific fullerenes. The numbering associated with trivial names is different, as it is based on principles like 'most reactive bond'. The two systems of numbering are shown below for three dimensional structures and Schlegel representations.

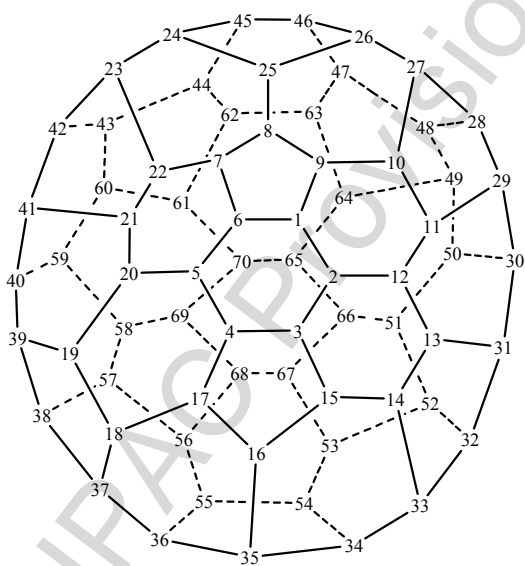


3-D Representation

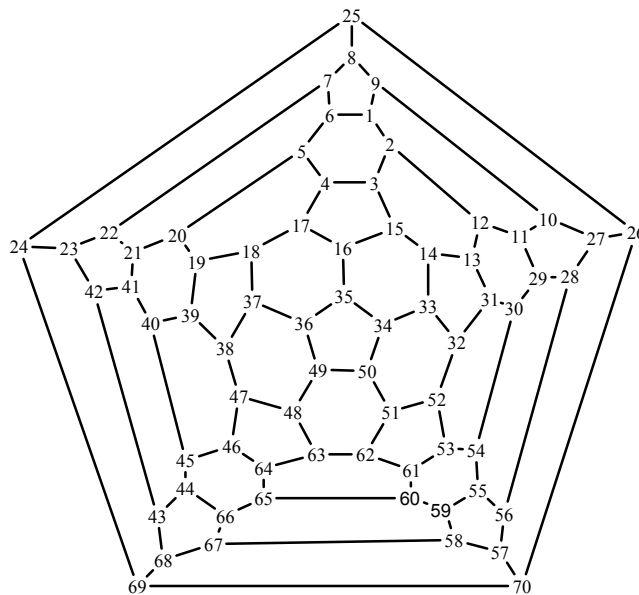


Schlegel representation

(C₆₀-I_h)[5,6]fullerene (systematic numbering) (PIN)

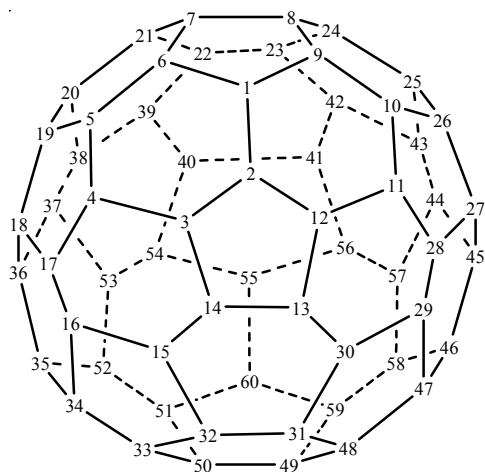


3-D Representation

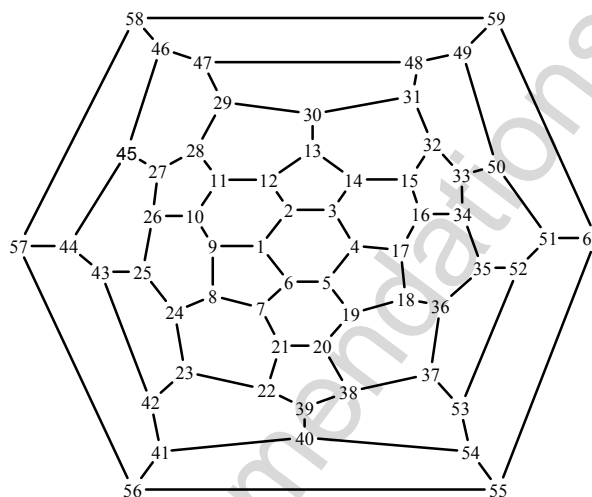


Schlegel representation

(C₇₀-D_{5h}(6))[5,6]fullerene (systematic numbering) (PIN)

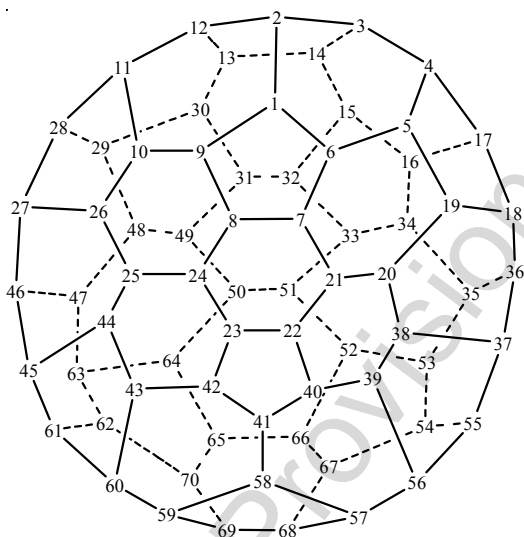


3-D Representation

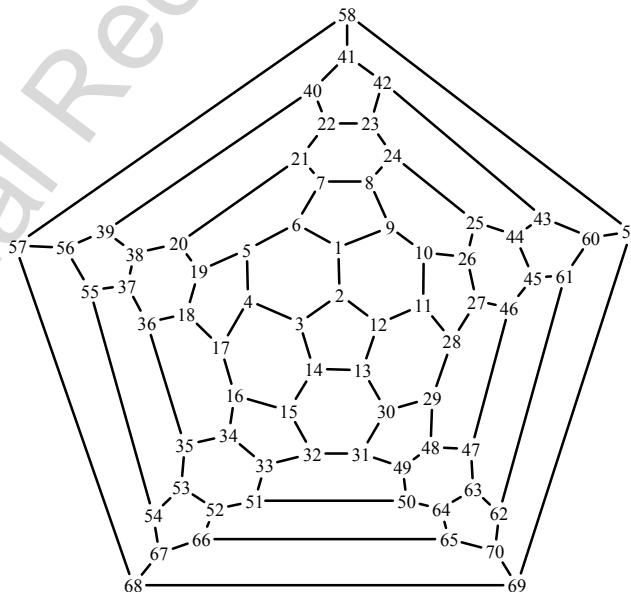


Schlegel representation

[60]fullerene (trivial numbering)



3-D Representation



Schlegel representation

[70- D_{5h}]fullerene (Trivial Numbering)

P-27.4 Structurally modified fullerenes

P-27.4.0 Introduction

P-27.4.1 Homofullerenes

P-27.4.2 Norfullerenes

P-27.4.3 Secofullerenes

P-27.4.4 Cyclofullerenes
P-27.4.5 Combination of operations

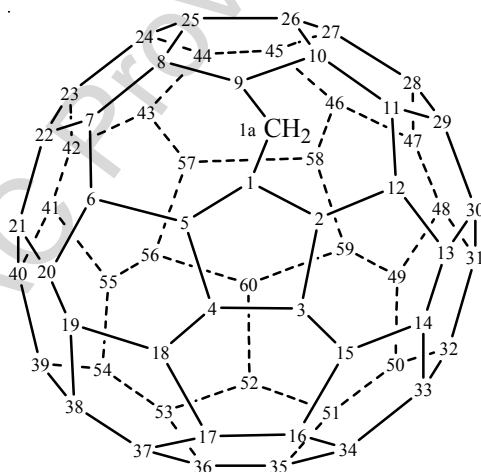
P-27.4.0 Introduction

The addition or removal of carbon atoms in a given fullerene does not create a new fullerene system described by a new number of carbon atoms and point group symbol, but is described by modifying the name of the unmodified fullerene using a nondetachable prefix, 'homo' or 'nor', respectively. In this way, fullerenes are parent structures analogous to fundamental structures used in the nomenclature of natural products (see Chapter 9). Similarly, the cleavage of a bond or the formation of new bonds in specific situations is expressed by using the nondetachable prefixes 'seco' and 'cyclo', respectively, which are also used in the nomenclature of natural products.

P-27.4.1 Homofullerenes

The replacement of a carbon-carbon bond of a fullerene by a methylene ($-\text{CH}_2-$) group is described by attaching the nondetachable prefix 'homo' to the name of the parent fullerene. The original numbering of the parent fullerene is retained. The location of the homo operation is described by a compound locant formed according to the method devised for insertion of a methylene group into a bond connector of a fundamental structure in the nomenclature of natural products (see P-93.2.2.2). The addition of two or more methylene groups is indicated by appropriate multiplying prefixes 'di', 'tri', etc. placed in front of the prefix 'homo'. The compound locant is formed by adding the letter 'a' (b', 'c', etc. if more than one methylene group replaces the bond) to the pair of locants which are the lowest locants consistent with the numbering of the fullerene, and enclosing the higher number in parentheses, for example '1(9)a'. Such compound locants must be used as locants for substituents or heteroatoms where there is ambiguity; where there is no ambiguity simple locants formed by adding the letter 'a' to the lowest locant, such as '1a' for the case above, may be used. Locants to denote the addition of methylene group(s) are differently used in the nomenclature of natural products (see P-93.2.2). Locants used by CAS are also different and must not be used to describe the replacement by methylene groups in preferred names of fullerenes (see Fu-4.1, ref. 10).

Example:



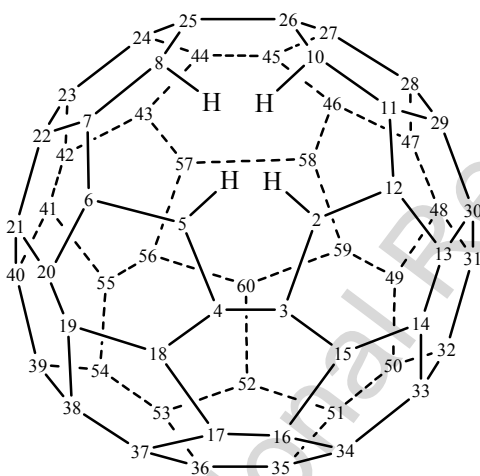
1aH-1(9)a-homo(C₆₀-I_h)[5,6]fullerene (PIN)

P-27.4.2 Norfullerenes

The nondetachable prefix 'nor' describes the deletion of carbon atoms from a fullerene structure; however, bonds attached to the atom removed are not reconnected as is the case in the nomenclature of natural products (see P-93.1). As a result, the connectivity of remaining atoms may be reduced from three to two, which requires the presence of hydrogen atoms. An even number of hydrogen atoms is implied in the name; if there is an odd number, one is expressed as indicated hydrogen because one carbon atom has changed from sp^2 to sp^3 hybridization. A connectivity of three may be satisfied by a heteroatom, such as nitrogen or boron and a connectivity of two by a heteroatom such as oxygen or sulfur; these heteroatoms are introduced in a separate operation. Locants for the atoms must be as low as possible.

The use of the 'nor' prefix in the nomenclature of natural products is not the same and must not be used in, or adapted to, fullerene nomenclature.

Example:

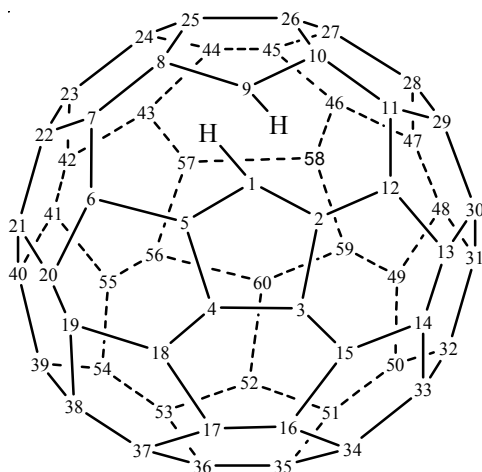


1,9-dinor(C_{60-I_h})[5,6]fullerene (PIN)

P-27.4.3 Secofullerenes

The nondetachable prefix 'seco' indicates the cleavage of fullerene bonds. Numbering of the parent fullerene is retained; where there is a choice, lowest possible locants are used to describe the seco operation. The valence requirements of the resulting carbon atoms with a connectivity of two are satisfied by hydrogen atoms following rearrangement of the double bonds. The hydrogen atoms are implied in the name of the secofullerene.

Example:



1,9-seco(C₆₀-I_h)[5,6]fullerene)PIN)

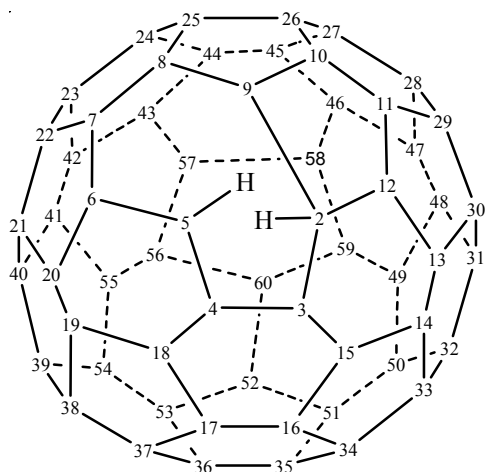
P-27.4.4 Cyclofullerenes

The nondetachable prefix ‘cyclo’ indicates the formation of a bond between two atoms of a modified fullerene or multifullerene structure. It almost always occurs in combination with one or more of the structure modifying prefixes ‘homo’, ‘nor’, and ‘seco’. No single fullerene is yet known that uses only ‘cyclo’. See the example under P-27.4.5.

P-27.4.5 Combination of structure modifying operations

When more than operation has been performed in a fullerene structure, the prefixes designating these operations are cited in names in the order cyclo, seco, homo, and nor in front of the name of the fullerene. This is the reverse order that the operation indicated by the prefix has for assignment of lowest locants. Nor prefixes are considered first for lowest locants and homo prefixes are senior to seco and cyclo for lowest locants since homo locants may be needed for the latter operations. Locants for cyclo and seco prefixes are determined by the lowest set of locants, then by the order of citation of the locants in the name.

Example:

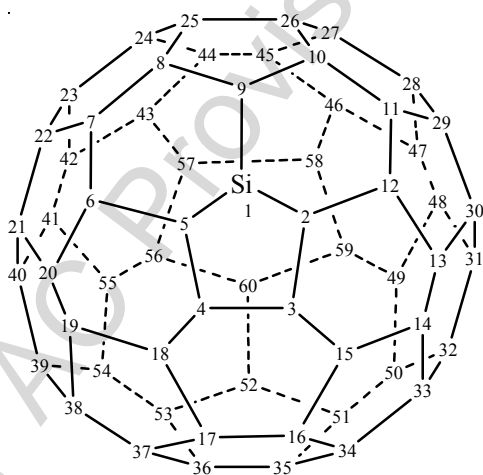


2H-2,9-cyclo-1-nor(C₆₀-I_h)[5,6]fullerene (PIN)

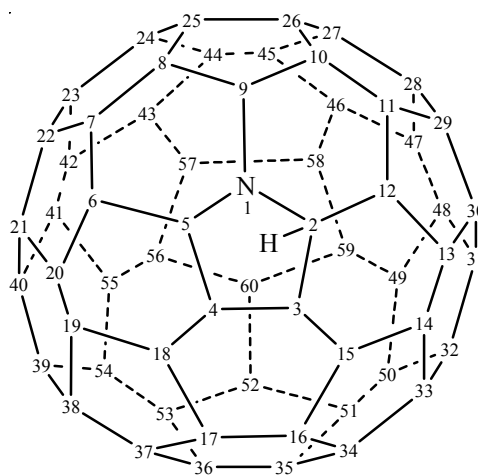
P-27.5 Replacement of skeletal atoms

P-27.5.1 Fullerenes in which carbon atoms have been replaced by one or more heteroatoms are called ‘heterofullerenes’. Skeletal replacement (‘a’) nomenclature is used to name fullerenes in which carbon atoms have been replaced by heteroatoms having standard bonding numbers according to the ‘a’ prefixes of organic replacement nomenclature (see P-15.4) or bonding numbers indicated by the λ -convention (see P-14.1). The parent name is ‘fullerene’ if double bonds are present or possible in the parent fullerene; if double bonds are not possible, the parent name is ‘fullerane’. The heteroatoms include all elements capable of being tricoordinate, including metals and semimetals. Replacement names for fullerenes in which all carbon atoms have been replaced by the same or different heteroatoms are preselected names (see P-12.2). Replacement of carbon atoms by trivalent heteroatoms may result in the need for indicated hydrogen.

Examples:



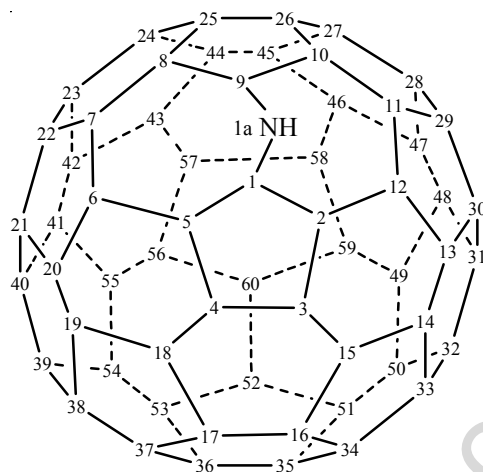
sila(C₆₀-I_h)[5,6]fullerene (PIN)



2H-1-aza(C₆₀-I_h)[5,6]fullerene (PIN)

P-27.5.2 When ‘homo’, ‘nor’, ‘seco’ or ‘cyclo’ prefixes co-occur with skeletal replacement terms, such as ‘oxa’ or ‘aza’, the replacement prefixes are cited in names in order of their seniority before structure modifying prefixes. Structure modifying prefixes are assigned low locants over replacement prefixes.

Example:



1aH-1a-aza-1(9)a-homo(C₆₀-I_h)[5,6]fullerene (PIN)

P-27.6 Addition of rings and ring systems to fullerenes

Addition of rings or ring systems to a fullerene is expressed as a *ortho* fusion operation, a bridging operation, or as a spirofusion operation as previously described in this Chapter.

P-27.6.1 Fullerenes *ortho* fused to organic rings or ring systems

P-27.6.2 Bridged fullerenes

P-27.6.3 Spirofullerenes

P-27.6.1 Fullerenes and modified fullerenes *ortho* fused to organic rings or ring systems

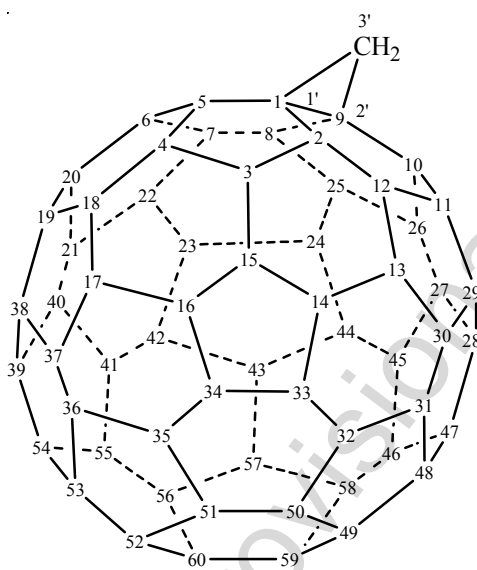
Fullerenes or modified fullerenes that share an adjacent pair of atoms with an organic ring or ring system are named by adapting the principles of fusion nomenclature described in Section P-25. As in normal organic fused ring systems, the pair of atoms shared by the fullerene or modified fullerene and the organic ring or ring system is regarded as part of both components. However, unlike normal fused systems, each component retains its own bonding pattern and numbering. Because of the nature of bonding in fullerenes, the fusion bond is always a single bond and the fusion atoms cannot accept an ‘exo’ double bond. After fusion, nonfullerene components other than alicyclic bi- and polycyclic ring systems have the maximum number of non cumulated double bonds and indicated hydrogen is cited as needed.

Organic rings and ring systems, including monocyclic rings and all polycyclic ring systems except spiro ring systems, are always cited as prefixes to the name of the fullerene or modified fullerene that is always the parent component. Each system retains its own name and numbering both for indicating fusion sites and for indicating positions of substitution. The fullerene or modified fullerene locants are always unprimed, and primes are added to the the fused organic rings or ring systems in

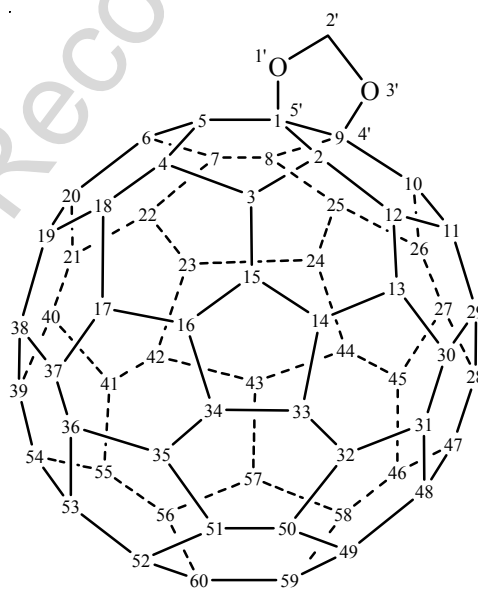
the order described below. The fusion is described by citing the primed locants of the organic ring or ring system component and the unprimed locants of the fullerene or modified fullerene in that order, enclosed in brackets and separated by a colon. Locants for monocyclic hydrocarbons are omitted in preferred IUPAC names.

The methodology used to name fused derivatives of fullerenes is also used for naming fused fundamental structures in the nomenclature of natural products (see P-97). It is important to note that it must be integrally applied as described to generate IUPAC names. CAS names are different and more in line with the normal fusion operation in which the parent component is the senior ring or ring system. When this approach must be used, CAS names of fullerenes and modified fullerenes must be used. Furthermore, it is possible to replace fusion operations by bridging operations, as for example, when the ring component is a cyclopropane or an oxirene ring. In these cases, bridging by using the bridging prefixes 'methano' or 'epoxy' (see P-25.4) can be an important alternative; it was recommended in the preliminary survey (see ref. 19). In general nomenclature, if this method is used, it must be associated with trivial fullerene names, including their specific numbering, to avoid any confusion with IUPAC names and numbering.

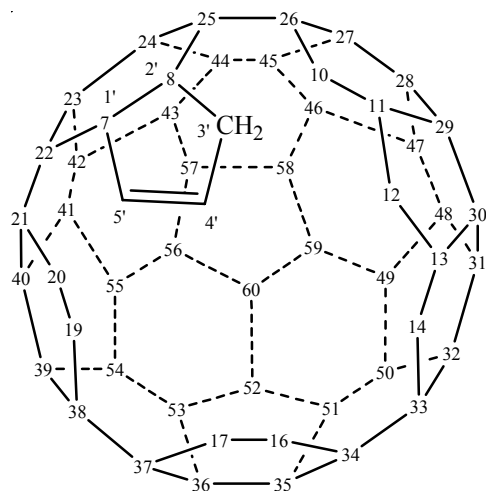
Examples:



3'*H*-cyclopropa[1,9](C₆₀-I_h)[5,6]fullerene (PIN)



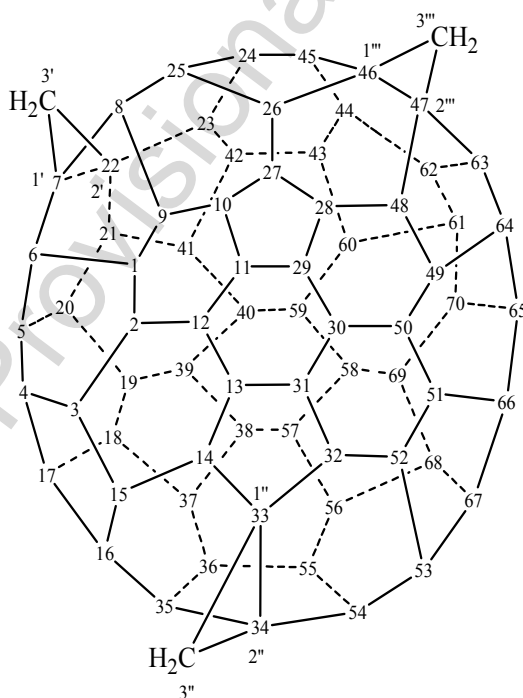
[1,3]dioxolo[4',5':1,9](C₆₀-I_h)[5,6]fullerene (PIN)



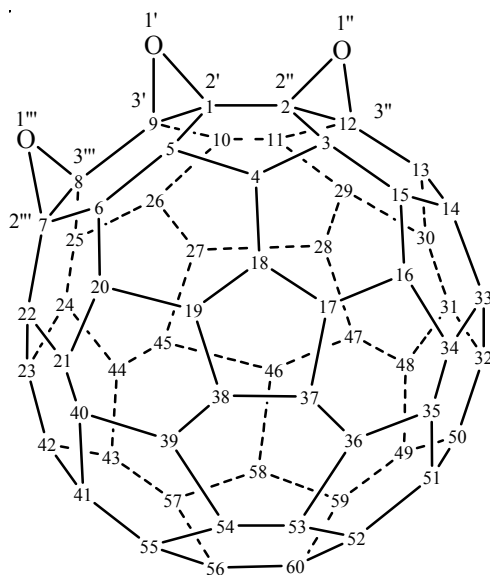
3'*H*-cyclopenta[7,8]-1,2,3,4,5,6,9,12,15,18-decanor(C_{60} - I_h)[5,6]fullerene (PIN)

When two or more of the same nonfullerene component are fused to a fullerene, primes are assigned according to the increasing value of the lower fullerene fusion locant. When different nonfullerene components are attached to a fullerene, primes are assigned in the alphanumerical order of the fusion prefix in the name reading from left to right, respecting the criterion for multiples of the same nonfullerene component just given. This methodology also applies to rings and ring systems fused to modified fullerenes.

Examples:



3'*H*,3''*H*,3'''*H*-tricyclopropa[7,22:33,34:46,47](C_{70} - I_h)[5,6]fullerene (PIN)

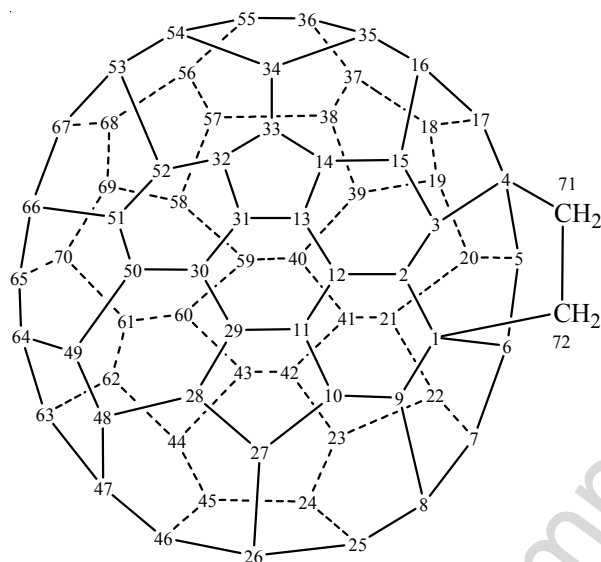


tris(oxireno)[2',3':1,9;2'',3'':2,12;2''',3''':7,8](C₆₀-I_h)[5,6]fullerene (PIN)

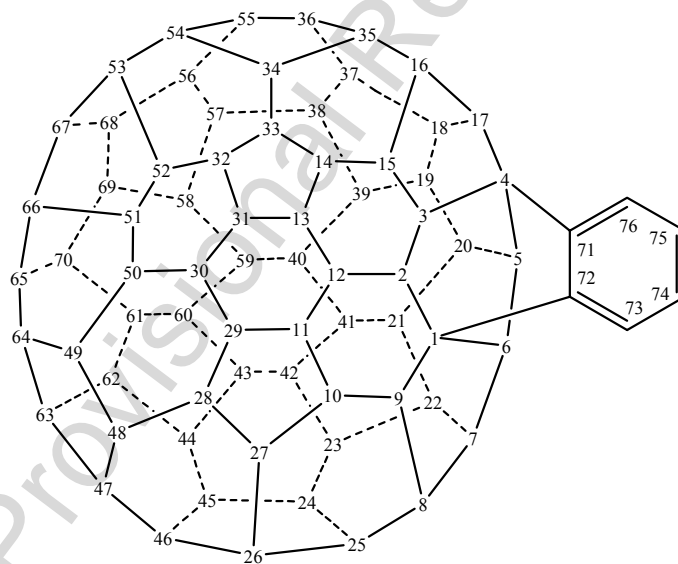
P-27.6.2 Bridged fullerenes

Bridges between nonadjacent atoms of a fullerene or modified fullerene are named and numbered according to established principles and rules for bridged fused ring systems (see P-25.4). Numbering of bridging atoms begins with the number following the highest number of the fullerene and starts with the atom adjacent to the fullerene atom with the higher locant number. Bridges between rings fused to fullerene and a parent fullerene, between two different rings fused to the same fullerene, or between two or more fullerenes joined by fused rings or ring systems are named using established bridge prefix names, but numbering begins with the bridge atom adjacent to the fused component with the least primed numbers and continues from this atom.

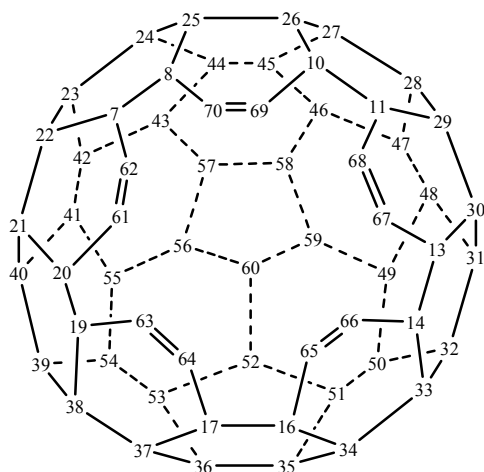
Examples:



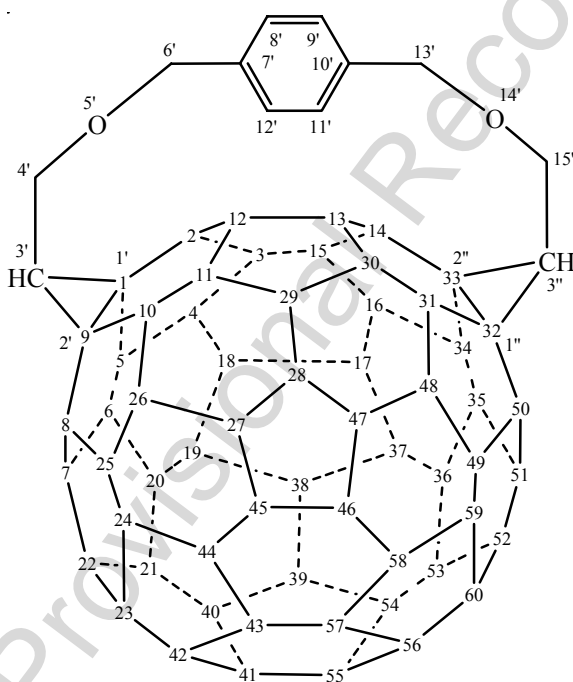
1,4-ethano(C_{70} - $D_{5h(6)}$)[5,6]fullerene (PIN)



1,4-[1,2]benzeno(C_{70} - $D_{5h(6)}$)[5,6]fullerene (PIN)



7,20:8,10:11,13:14,16:17,19-pentaetheno-1,2,3,4,5,6,9,12,15,18-decanor(C₆₀-I_h)[5,6]fullerene (PIN)



3',3''-(methanooxymethano[1,4]benzenomethanooxymethano)-
3'H,3''H-dicyclopropa[1,9:32,33] (C₆₀-D_{5h(6)})[5,6]fullerene (PIN)

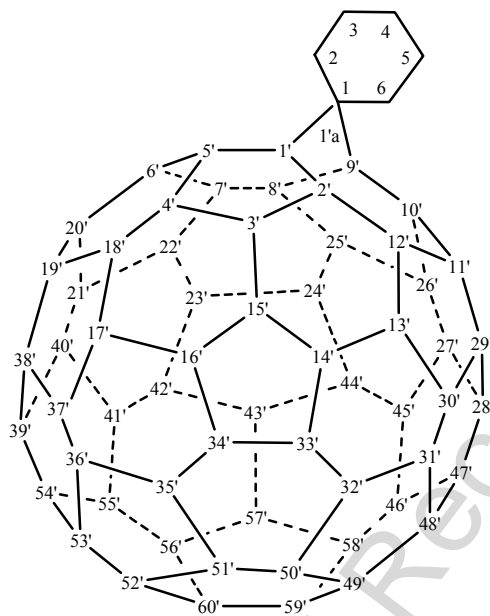
P-27.6.3 Spiro fullerenes

Fullerenes cannot themselves form spiro compounds directly due to their specific connectivity and, as mentioned earlier, spiro ring systems are not fused to fullerenes.

Spiro fullerenes formed from homofullerenes and fullerenes fused to organic ring or ring systems follow the normal procedure for naming organic spiro systems that contain at least one polycyclic

ring system, as described in P-24.5. Spiro fullerene parent hydrides will not necessarily have unprimed numbers as locants, as the alphanumeric order is used to name this type of spiro compound.

Example:



spiro[cyclohexane-1,1'-[1aH-1(9)a]-homo(C₆₀-I_h)[5,6]fullerene] (PIN)

P-28 Ring assemblies

- P-28.0 Introduction
- P-28.1 Definitions
- P-28.2 Ring assemblies of two identical cyclic systems
- P-28.3 Unbranched ring assemblies of three or more identical cyclic systems
- P-28.4 Ring assemblies of identical cyclic systems with indicated hydrogen atom(s)
- P-28.5 Ring assemblies of cyclic systems modified by skeletal replacement ('a') nomenclature
- P-28.6 Branched ring assemblies of identical cyclic systems
- P-28.7 Ring assemblies of nonidentical cyclic systems

P-28.0 Introduction

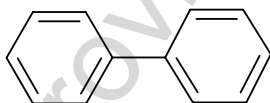
Assemblies of cyclic parent hydrides linked by single or double bonds are described in this Section. They are named by using the so-called 'Latin multiplying prefixes', 'bi', 'ter', 'quater', etc. to indicate the number or rings or ring systems in the assembly.

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.

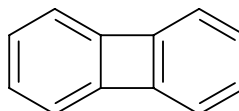
Names of substituent groups described further in Section 29 are used in this Section.

P-28.1 Definitions

Two or more cyclic systems (single rings or fused systems, alicyclic von Baeyer systems, spiro systems, phane systems, fullerenes) that are directly joined to each other by single or double bonds are called 'ring assemblies' when the number of such direct ring junctions is one less than the number of cyclic systems involved.

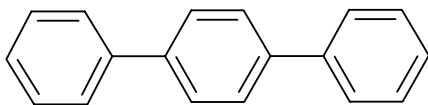


a ring assembly

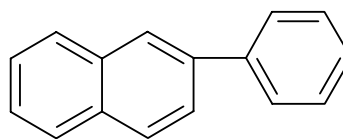


a fused ring system

Ring assemblies are composed of identical cyclic systems (rings or ring systems); assemblies of nonidentical cyclic systems (rings or ring systems) are not called ring assemblies for the purposes of organic nomenclature, for example:



three identical rings
(a ring assembly)



two different ring systems

P-28.2 Ring assemblies of two identical cyclic systems with no indicated hydrogen atoms

P-28.2.1 Ring assemblies with a single bond junction

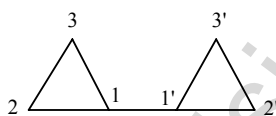
Assemblies of two identical cyclic systems joined by a single bond are named by one of two methods:

- (1) by placing the prefix 'bi' before the name of the corresponding parent hydride enclosed in parentheses, if necessary. Parentheses are used to avoid confusion with von Baeyer names;
- (2) by placing the prefix 'bi' before the name of the corresponding substituent group (for names of substituent groups, see P-29), enclosed in parentheses, if necessary.

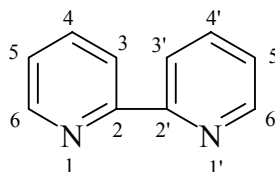
Except for biphenyl, for which method (2) is used, method (1) leads to preferred IUPAC names.

Each cyclic system is numbered in the usual way, one with unprimed locants, the other with primed locants, indicating the positions of attachment. Lowest possible locants must be used to denote the positions of attachment.

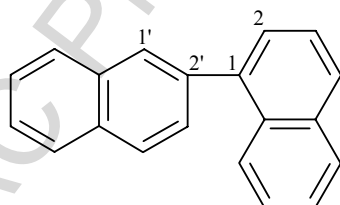
Examples:



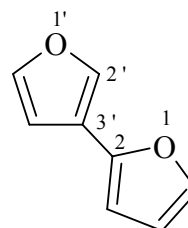
- (1) 1,1'-bi(cyclopropane) (PIN)
- (2) 1,1'-bi(cyclopropyl)



- (1) 2,2'-bipyridine (PIN)
- (2) 2,2'-bipyridyl



- (1) 1,2'-binaphthalene (PIN)
- (2) 1,2'-binaphthyl

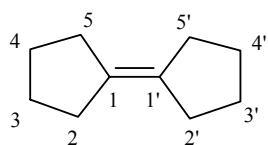


- (1) 2,3'-bifuran (PIN)
- (2) 2,3'-bifuryl

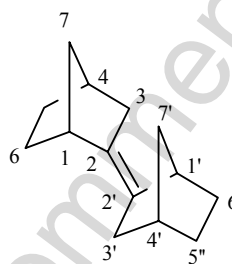
P-28.2.2 Ring assemblies with a double bond junction

When two cyclic systems are linked by a double bond, method (2) described in P-28.2.1 is the sole method recommended. Method (2) has also been used in which the presence of a double bond was indicated by the Greek letter Δ and the point of attachment of the ring was given by superscript locants numbers. This method is not continued in these recommendations; accordingly, ring assemblies of three or more identical cyclic systems interconnected by double bonds must be named by other methods (see P-31).

Examples:

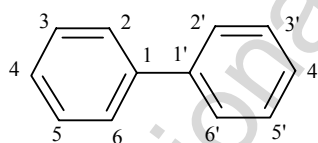


1,1'-bi(cyclopentylidene) (PIN)
(not $\Delta^{1,1'}$ -bicyclopentylidene)



2,2'-bi(bicyclo[2.2.1]heptan-2-ylidene) (PIN)
(not $\Delta^{2,2'}$ -bicyclo[2.2.1]heptanylidene)

P-28.2.3 A ring assembly composed of two benzene rings is named by method (2) described in P-28.2.1; locants are required for the IUPAC preferred name.



1,1'- biphenyl (PIN)
biphenyl

P-28.3 Unbranched ring assemblies consisting of three or more identical cyclic systems

P-28.3.1 Unbranched ring assemblies consisting of three or more identical cyclic systems are named by placing an appropriate numerical prefix 'ter-', 'quater-', 'quinque-', etc. before the name of the parent hydride corresponding to the repetitive unit. Exceptionally, ring assemblies composed of three or more benzene rings are named by using the term 'phenyl'. For phane names, where appropriate, see P-26)

Assemblies of three or more identical cyclic systems may be numbered by one of the two following methods. Method (a) is used for preferred IUPAC names.

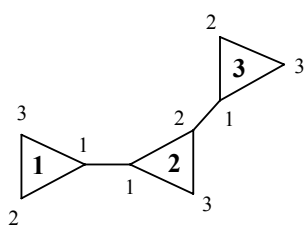
- Each cyclic system of the assembly is numbered consecutively and each ring or ring system is numbered in its usual way. Composite locants (see P-14.3.1) are formed by citing the locants denoting positions in each ring or ring system as superscripts to the locants indicating the position of a cyclic system in the assembly (ref. 20). Points of

attachment are assigned the lowest possible locants. For another possible numbering system, see ref. 21.

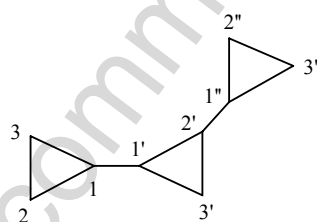
- (b) Unprimed locants are assigned to one of the terminal cyclic systems, the other cyclic systems being primed serially. Points of attachment are assigned the lowest locants possible; unprimed numbers are lower than primed.

Locants indicating points of attachment are placed before the name of the assembly, in ascending order; locants denoting junctions are separated by a comma and sets of junction locants are separated by a colon.

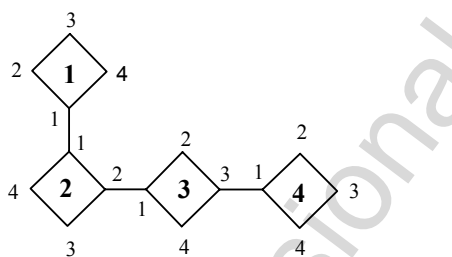
Examples (the number in parentheses reflects the method given in P-28.2.1; the letter reflects the numbering method given in P-28.3.1):



(1a) 1¹,2¹:2²,3¹-tercyclopropane (PIN)



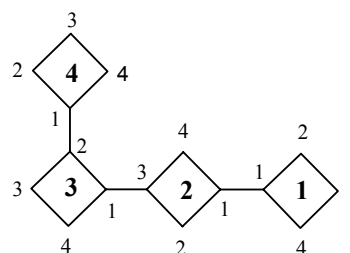
(1b) 1,1':2',1''-tercyclopropane



(1a) 1¹,2¹:2²,3¹:3³,4¹-quatercyclopropane (PIN)

correct numbering

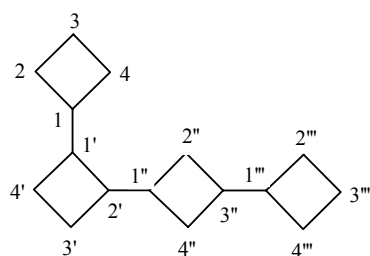
not



(1b) 1¹,2¹:2³,3¹:3²,4¹-quatercyclopropane

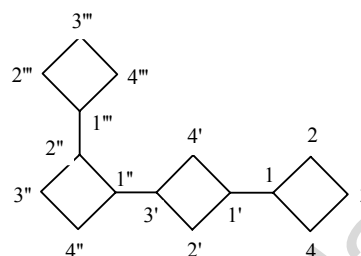
incorrect numbering

(the locant set 1¹,2¹:2²,3¹:3³,4¹ in 1a is lower than the locant set 1¹,2¹:2³,3¹:3²,4¹ in 1b)

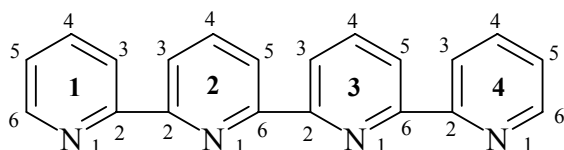


(1b) 1,1':2',1'':3'',1'''-quatercyclobutane
 correct numbering

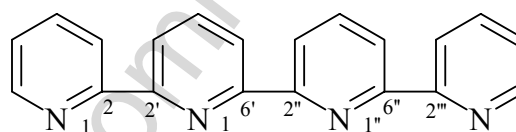
(the locant set 1,1':2',1'':3'',1''' in 2a is lower than 1,1':3',1'':2'',1''' in 2b)



(1b) 1,1':3',1'':2'',1'''-quatercyclobutane
 incorrect numbering



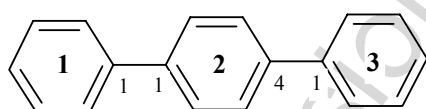
(1) 1²,2²:2⁶,3²:3⁶,4²-quaterpyridine (PIN)



(2) 2,2':6',2'':6'',2'''-quaterpyridine

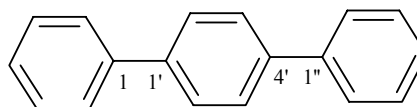
P-28.3.2 As exceptions to the use of parent hydride names, the names terphenyl, quaterphenyl, etc. are used.

Examples (the numerical number reflects the method given in P-28.2.1; the letter the numbering method given in P-28.3.1):

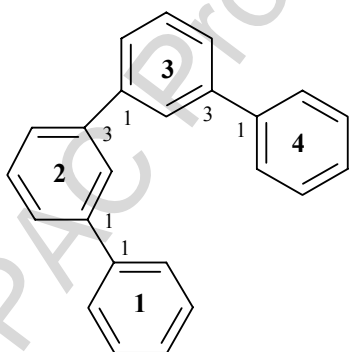


(2a) 1¹,2¹:2⁴,3¹-terphenyl (PIN)

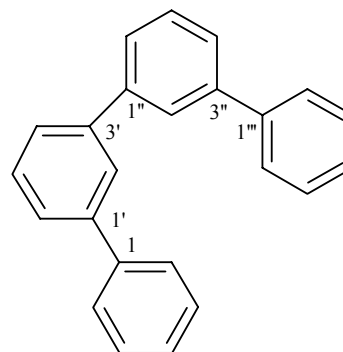
or



(2b) 1,1':4',1''-terphenyl
p-terphenyl



(2a) 1¹,2¹:2³,3¹:3³,4¹-quaterphenyl (PIN)



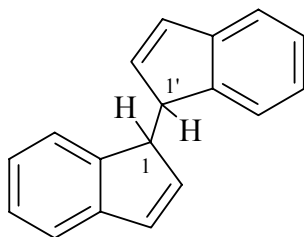
(2b) 1,1':3',1'':3'',1'''-quaterphenyl
m-quaterphenyl

P-28.4 Ring assemblies of identical cyclic systems with indicated hydrogen atom(s)

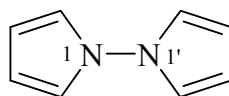
P-28.4.1 Ring assemblies are named and numbered according to P-28.2 and P-28.3 ignoring the indicated hydrogen atoms of the rings or ring systems. The maximum number of double bonds is added taking into account the junction positions. Any remaining saturated ring positions are designated as indicated hydrogen, placed together with the appropriate locant(s) at the front of the name of the assembly.

The citation of indicated hydrogen, if needed, at the front of the name of the ring assembly is a change from previous practice where indicated hydrogen was kept with the name of the individual ring, for example, 2,2'-bi-2*H*-pyran. This required that the indicated hydrogen had to be able to be at the same position in each ring of the ring assembly, as in 2,3'-bi-1*H*-indole. By citing the indicated hydrogen in front of the name of the ring assembly, which follows the new procedure for naming bridged fused systems (see P-25.7.1.3.2) and spiro ring systems (see P-24.3.2) that utilize indicated hydrogen, more assemblies of rings can be treated as ring assemblies, for example, 1*H*,2'*H*-2,4'-biindene. The advantages of this method become more obvious when naming derivatives such as a ketone or bivalent

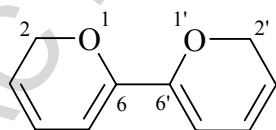
Examples:



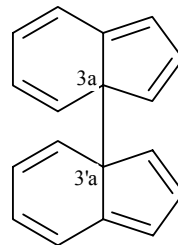
1*H*,1'*H*-1,1'-biindene (PIN)
(not 1,1'-bi-1*H*-indene)



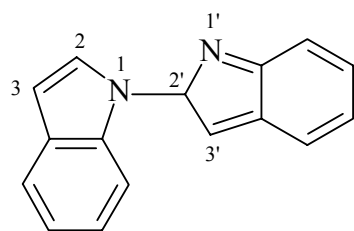
1,1'-bipyrrole (PIN)
(no indicated hydrogen needed)
(not 1,1'-bi-1*H*-pyrrole)



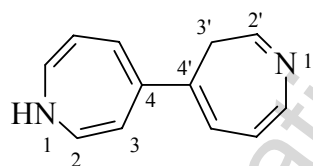
2*H*,2'*H*-6,6'-bipyran (PIN)
(not 6,6'-bi-2*H*-pyran)



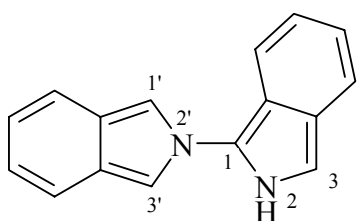
3*a*,3'*a*-biindene
(no indicated hydrogen needed)
(not 3*a*,3'*a*-bi-3*aH*-indene)



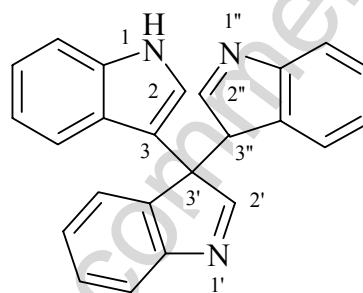
1,2'-biindole (PIN)
 (no indicated hydrogen needed)



1H,3'H-4,4'-biazepine (PIN)



2H-1,2'-biisindole (PIN)

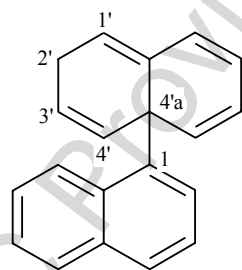


1²H-1³,2³:2³,3³-terindole (PIN)
 1H-3,3':3',3''-terindole

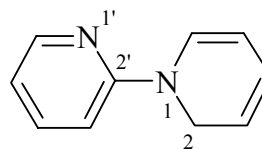
P-28.4.2 Ring assemblies of identical cyclic systems requiring added hydrogen

The 'added hydrogen method' (see P-14.6) is used when needed to accommodate the junction of the valence bond. The added hydrogen symbol is enclosed in parentheses and placed immediately after the locant of the point of attachment of the junction bond to which it relates.

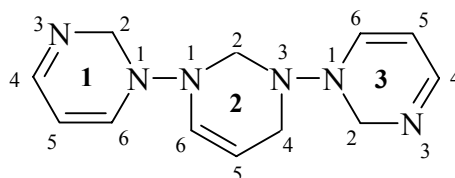
Examples:



1,4'a (2'H)-binaphthalene (PIN)

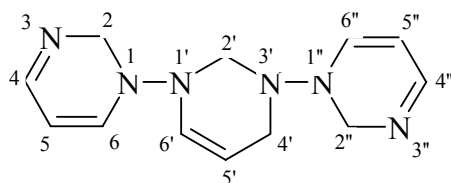


1(2H),2'-bipyridine (PIN)



$1^1,2^1(1^2H,2^2H):2^3,3^1(2^4H,3^2H)$ -terpyrimidine (PIN)
 [name method (1), P-28.2.1; numbering method (a), P-28.3.1]

or

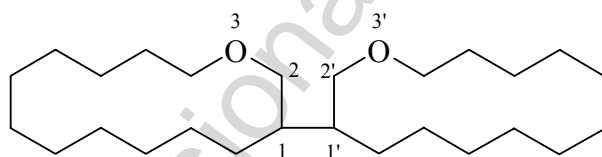


$1,1'(2H,2'H):3',1''(4'H,2''H)$ -terpyrimidine
 [name method (1), P-28.2.1; numbering method (b), P-28.3.1]

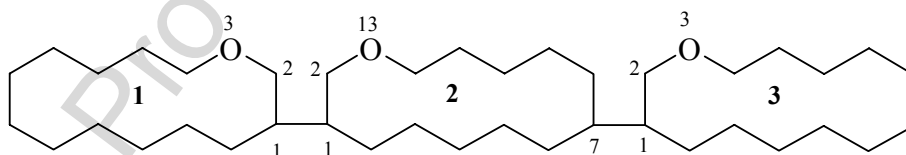
P-28.5 Ring assemblies composed of identical cyclic systems modified by skeletal replacement ('a') nomenclature

P-28.5.1 Assemblies composed of identical heterocyclic compounds are named by using the names of parent hydrides, except in the case of heterocyclic compounds of the von Baeyer type and of monocyclic compounds having more than 10 members that are named by using skeletal replacement ('a') nomenclature. In this case, the 'a' prefixes are placed at the front of the name of the hydrocarbon ring assembly.

Examples:

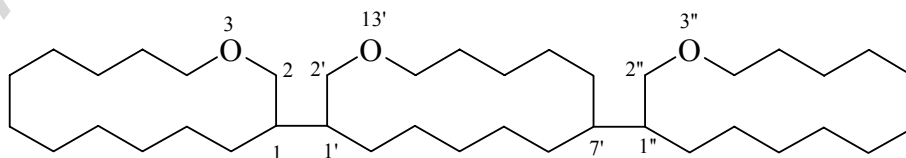


$1,1'$ -dioxo- $3,3'$ -bi(cyclotetradecane) (PIN)

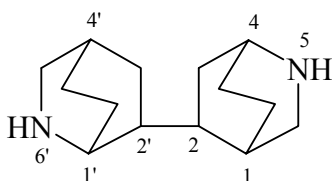


$1^3,2^{13},3^3$ -trioxa- $1^1,2^1:2^7,3^1$ -tercyclotetradecane (PIN)
 [name method (1), P-28.2.1; numbering method (a), P-28.3.1]

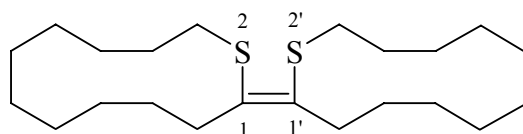
or



3',3'',13'-trioxa-1,1':7',1''-tercyclo[2.2.2]decane
 [name method (1), P-28.2.1; numbering method (b), P-28.3.1]



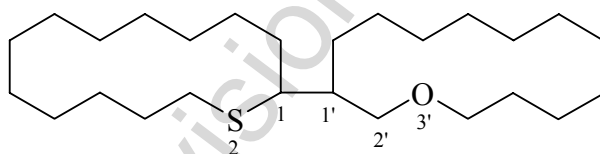
5,6'-diazabicyclo[2.2.2]octane (PIN)



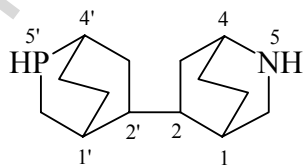
2,2'-dithia-1,1'-bi(cyclododecan-2-ylidene) (PIN)

P-28.5.2 Since hydrocarbon ring assemblies are the parent structures for the application of skeletal replacement ('a') nomenclature, heteroatoms do not need to be identical or present in the same number. When heteroatoms of different elements are present, normal skeletal replacement ('a') nomenclature is used to name the heterocycles. Low locants are assigned to heteroatoms as a set, then in the order: O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Examples:



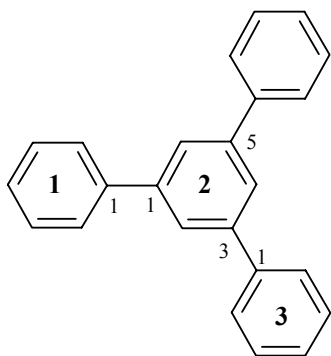
3'-oxa-2-thia-1,1'-bi(cyclotetradecane) (PIN)
 [not 3-oxa-2'-thia-1,1'-bi(cyclotetradecane)]
 (the locant set 2,3' is lower than 3,2')



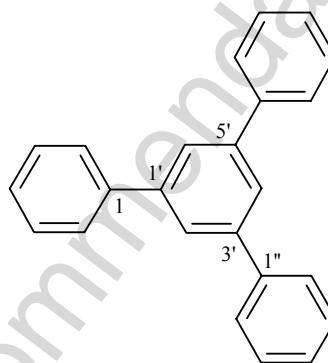
5-aza-5'-phospha-2,2'-bibicyclo[2.2.2]octane (PIN)
 (not 5'-aza-5-phospha-2,2'-bibicyclo[2.2.2]octane)
 (the locant 5 is lower than 5' and the prefix 'aza' has priority to be assigned the lower locant)

P-28.6 Branched ring assemblies of identical cyclic systems are named by substituting the longest unbranched assembly. The names of substituent groups are formed in accord with the methods described in P-29.3.5 and 29.6.1. If necessary, the criteria for selecting the principal chain are applied: longest chain, maximum number of substituents, lowest locants for substituents considered together, then in alphanumerical order.

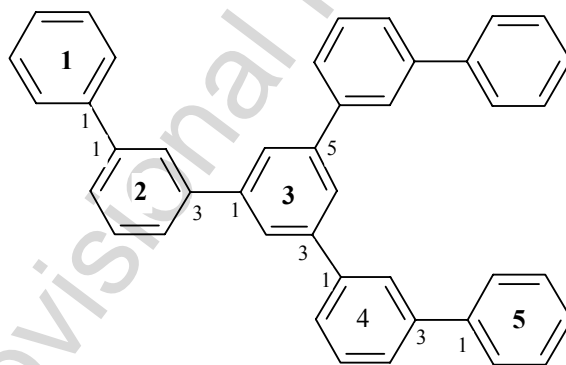
Examples:



2⁵-phenyl-1¹,2¹:2³,3¹-terphenyl (PIN)
 [name method (2), P-28.2.1;
 numbering method (a), P-28.3.1]

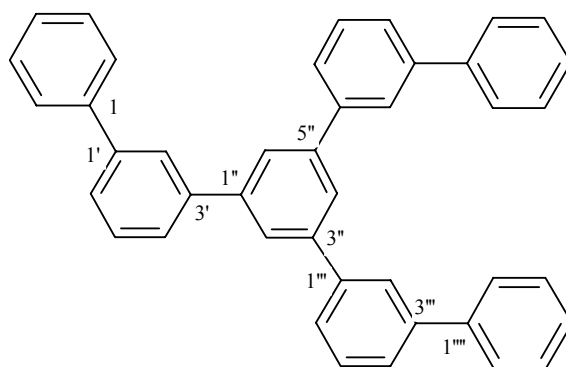


5'-phenyl-1,1':3',1''-terphenyl
 [name method (2), P-28.2.1;
 numbering method (b), P-28.3.1]

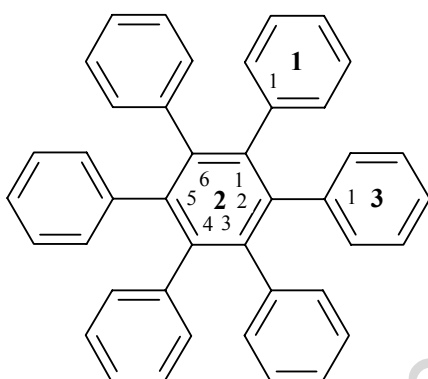


3⁵-(biphenyl-3-yl)-1¹,2¹:2³,3¹:3³,4¹:4³,5¹-quinquephenyl
 [name method (2), P-28.2.1; numbering method (a), P-28.3.1]

or

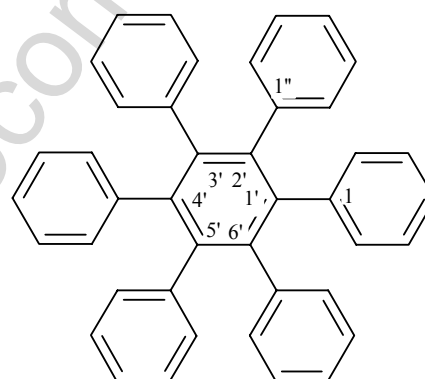


5''-(biphenyl-3-yl)-1,1':3'1'':3''-1''':3'''-1''''-quinquephenyl
 [name method (2), P-28.2.1; numbering method (a), P-28.3.1]



2³,2⁴,2⁵,2⁶-tetraphenyl-1¹,2¹:2²,3¹-terphenyl (PIN)
 [name method (2), P-28.2.1;
 numbering method (a), P-28.3.1]

or



3',4',5',6'-tetraphenyl-1,1':2',1''-terphenyl
 [name method (2), P-28.2.1;
 numbering method (b), P-28.3.1]

P-28.7 Assemblies of nonidentical cyclic systems

Assemblies of cyclic systems that cannot be treated as ring assemblies as described above (P-28.1 and P-28.2) are simply nonidentical assemblies and are named by regular substitutive nomenclature principles. Such cyclic hydrocarbon assemblies are discussed in Section P-61.2.1 and nonidentical cyclic assemblies containing heteroatoms, such as Si, N, B, in Section 68. Phane nomenclature (see P-26), where applicable, is used to name ring assemblies composed of identical or nonidentical cyclic systems.

Ring assemblies of identical cyclic systems that are partially unsaturated or partially saturated can be modified either by the endings 'ene' or 'yne' (introduction of double bonds in saturated systems) or by using the prefixes 'hydro/dehydro' in mancude systems (see Section P-31). In some cases, especially in the case of benzene ring assemblies, assemblies of nonidentical cyclic systems result from such operations.

P-29 Prefixes denoting substituent groups derived from parent hydrides

- P-29.0 Introduction
- P-29.1 Definitions
- P-29.2 General methodology for forming systematic names
- P-29.3 Systematic names of substituents derived from parent hydrides
- P-29.4 Complex substituent groups
- P-29.5 Compound groups
- P-29.6 Retained names

P-29.0 Introduction

This Section includes the names of substituent groups derived from the parent hydrides described in Sections P-21 to P-28 and used as prefixes in substitutive nomenclature. The methodology for forming systematic names is fully described in this Section; the selection of preferred names is treated in Chapter 5, Section P-56.

P-29.1 Definitions

Prefixes derived from parent hydrides are used in many ways in the nomenclature of organic compounds and may be classified as simple prefixes, compound prefixes, and complex prefixes. The definitions given below differ from those that were previously recommended (see A-2.3 in ref. 1 and R-4.1 in ref. 2).

P-29.1.1 A simple substituent group has a name consisting of one part that describes an atom or group of atoms as a unit. Normally, the basic multiplying prefixes 'di', 'tri', 'tetra', etc, denote the presence of more than one identical simple substituent group in a compound, but see P-16.3.

P-29.1.2 A compound substituent group consists of a simple substituent group (the parent substituent group) to which is attached one or more simple substituent groups. Compound substituent group names are formed by combining the names of two or more simple substituent groups. There are two ways to do this:

- (1) by an additive operation
- (2) by the substitutive operation

Names for compound substituent groups are formed by the substitution operation rather than by an additive operation unless the simple parent substituent group does not have a name that is acceptable for substitution. Compound substituent groups formed by substitution are cited in names as prefixes, often called 'substituted prefixes'. Compound substituent groups formed by addition are cited in names as prefixes, often called 'concatenated prefixes'. Derived multiplying prefixes 'bis', 'tris', 'tetrakis' are used to multiply compound prefixes and to avoid ambiguity when the basic multiplying prefixes are already part of the name of a parent hydride (see P-16.3).

P-29.1.3 A complex substituent group consists of a parent substituent group to which is attached at least one compound substituent group. In a complex substituent group, the parent substituent group of a component compound substituent group is called a subsidiary parent substituent group. Multiplicative prefixes, used as central part in multiplicative nomenclature (see P-15.3.2.3), are

formed by the additive operation and when they consist of three or more parts are often considered as 'complex concatenated prefixes'.

P-29.2 General methodology for naming substituent groups

The presence of free valences formally derived from the loss of one or more hydrogen atoms from a parent hydride are denoted by suffixes 'yl', 'ylidene', and 'ylidyne', together with the multiplying prefixes indicating the number of free valences; lowest locants are assigned to all free valences as a set, then in the order 'yl', 'ylidene', 'ylidyne'. In names, the suffixes are cited in the order 'yl', 'ylidene', 'ylidyne'. In these recommendations, the suffixes 'ylidene' and 'ylidyne' are used only to indicate the attachment of a substituent to a parent hydride or parent substituent by a double or triple bond, respectively.

Systematic names are formed by using the suffixes 'yl', 'ylidene' and 'ylidyne', with elision of the final letter 'e' of parent hydrides, when present, according to two methods as follows:

Monovalent	Divalent	Trivalent	Tetravalent	etc.
-yl	-diyl -ylidene	-triyl -ylidyne -ylidene	-tetrayl -ylidyne -diylidene -diylidene	etc.

P-29.2.1 Specific method. The suffixes 'yl', 'ylidene', and 'ylidyne' replace the ending 'ane' of the parent hydride name. The atom with the free valence terminates a chain and always has the locant '1', which is omitted from the name. This method is recommended only for saturated acyclic and monocyclic hydrocarbon substituent groups and for the mononuclear hydrides of silicon, germanium, tin, and lead.

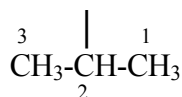
The specific method is no longer applicable to boron.

Examples:

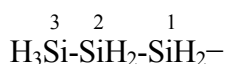
CH_3-	methyl (PIN)	$\text{C}_6\text{H}_{11}-$	cyclohexyl (PIN)
SiH_3-	silyl (PIN)	$\text{CH}_3-\text{CH}_2-\text{CH}=\text{}$	propylidene (PIN)
$\text{CH}_2=\text{}$	methylidene (PIN)	$\text{CH}_3-\text{C}\equiv\text{}$	ethylidyne (PIN)

P-29.2.2 General method. Any of the suffixes 'yl', 'ylidene', and 'ylidyne' is added to the name of the parent hydride with elision of the terminal letter 'e', if present, when followed immediately by the letter 'y'. The locants for the atoms of free valences are as low as is consistent with any established numbering of the parent hydride and except for mononuclear parent hydrides or the suffix 'ylidyne', the locant '1' must be cited.

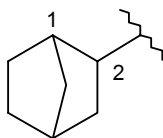
Examples:



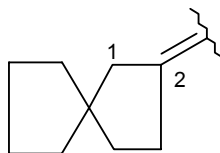
propan-2-yl (PIN)



trisilan-1-yl (PIN)



bicyclo[2.2.1]heptan-2-yl (PIN)



spiro[4.4]nonan-2-ylidene (PIN)

P-29.3 Systematic names of substituents derived from saturated parent hydrides

P-29.3.1 Substituent groups derived from mononuclear parent hydrides

P-29.3.2 Substituent groups derived from acyclic parent hydrides

P-29.3.3 Substituent groups derived from saturated cyclic parent hydrides

P-29.3.4 Substituent groups derived from mancude parent hydrides

P-29.3.5 Substituent groups derived from ring assemblies

P-29.3.5 Substituent groups derived from phane names

P-29.3.1 Substituent groups derived from mononuclear hydrides

Substituent groups are formed by applying the specific method, P-29.2.1, to the mononuclear parent hydrides of carbon, silicon, germanium, tin, and lead (boron is no longer included); the general method, P-29.2.2, is applied to other mononuclear parent hydrides with the exception of oxygen. Thus, method P-29.2.2 is limited to mononuclear hydrides containing S, Se, Te, N, P, As, Sb, Bi, B, Al, Ga, In, and Tl.

This rule is more restrictive than Rule 2.5 cited in the Guide (ref. 2) because it is not necessary to generate names that are not used as preferred names, nor used to generate those of complex substituent groups, as indicated in Section P-29.4 below. The prefixes boryl, borylidene and borylidyne have been replaced by boranyl, boranylidene,, and boranylidyne, respectively

Examples:

$\text{CH}_3\text{-}$
methyl (PIN)

$\text{GeH}_3\text{-}$
germyl (PIN)

$\text{BH}_2\text{-}$
boranyl (PIN)
(not boryl)

$\text{CH}_2=$ methylidene (PIN)	$\text{SnH}_2=$ stannylidene (PIN)	$\text{BH}=$ boranylidene (PIN) (not borylidene)
$\text{SH}-$ sulfanyl (PIN) (no longer mercapto)	PH_2- phosphanyl (PIN) (not phosphino)	AlH_2- alumanyl (PIN)
$\text{S}=$ sulfanylidene (PIN) thioxo	$\text{AsH}=$ arsanylidene (PIN) (not arsinidine)	$\text{AlH}=$ alumanylidene (PIN)

P-29.3.2 Substituent groups derived from acyclic parent hydrides

Names of substituent groups are derived from those of the acyclic parent hydride and formed by the specific and general methods described in P-29.2.

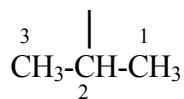
P-29.3.2.1 The specific method P-29.2.1 generates 'alkyl', 'alkylidene', and 'alkylidyne' substituent groups. The free valences denoted by the suffixes 'yl', 'ylidene', and 'ylidyne' are always situated at an extremity of the chain that is assigned the locant 1. This locant is omitted in names.

Examples:

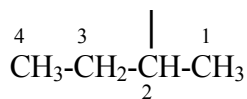
$\overset{2}{\text{CH}_3}-\overset{1}{\text{CH}_2}-$	ethyl (PIN)
$\overset{3}{\text{CH}_3}-\overset{2}{\text{CH}_2}-\overset{1}{\text{CH}_2}-$	propyl (PIN)
$\overset{4}{\text{CH}_3}-\overset{3}{\text{CH}_2}-\overset{2}{\text{CH}_2}-\overset{1}{\text{CH}_2}-$	butyl (PIN)
$\overset{3}{\text{CH}_3}-\overset{2}{\text{CH}_2}-\overset{1}{\text{CH}}=$	propylidene (PIN)
$\overset{4}{\text{CH}_3}-\overset{3}{\text{CH}_2}-\overset{2}{\text{CH}_2}-\overset{1}{\text{C}}\equiv$	butylidyne (PIN)

P-29.3.2.2 The general method, P-29.2.2, is used to generate names of substituent groups other than those described in P-29.3.2.1. In contrast to alkyl, alkylidene, and alkylidyne groups in carbon compounds, those substituents named by the general method P-29.2.2 are called 'alkanyl', 'alkanylidene', 'alkanylidyne', 'alkanediyl', 'alkanylylidene', etc., substituent groups. Low locants are assigned to free valences considered as a set, in accordance with the numbering of the chain. If there is a choice, low locants are assigned, in order, to the suffixes 'yl', 'ylidene', and 'ylidyne'. In names, the suffixes are cited in the order 'yl', 'ylidene', and 'ylidyne'.

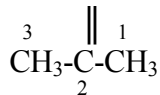
Examples:



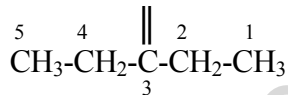
propan-2-yl (PIN)



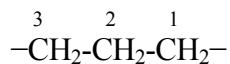
butan-2-yl (PIN)



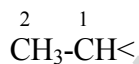
propan-2-ylidene (PIN)



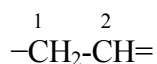
pentan-3-ylidene (PIN)



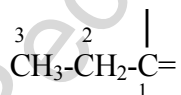
propane-1,3-diyl (PIN)



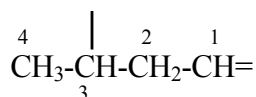
ethane-1,1-diyl (PIN)



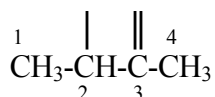
ethan-1-yl-2-ylidene (PIN)



propan-1-yl-1-ylidene (PIN)



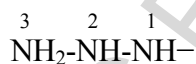
butan-3-yl-1-ylidene (PIN)



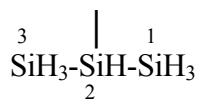
butan-2-yl-3-ylidene (PIN)

AsH₃-AsH₂-
diarsanyl (PIN)

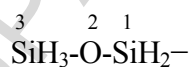
SiH₃-SiH₂-
disilanyl (PIN)



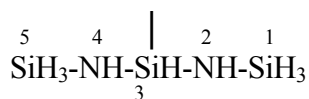
triazan-1-yl (PIN)



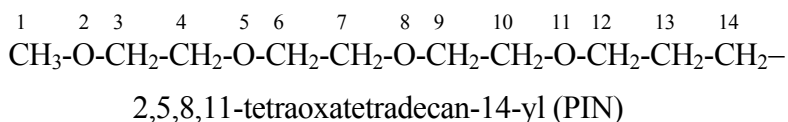
trisilan-2-yl (PIN)



disiloxanyl (PIN)



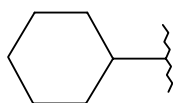
trisilazan-3-yl (PIN)



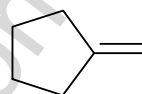
P-29.3.3 Substituent groups derived from saturated cyclic parent hydrides

With the exception of substituent groups derived from cycloalkanes that are named by the specific method P-29.2.1 only, all other substituent groups derived from saturated cyclic parent hydrides are named by the general method, P-29.2.2. Low locants are assigned to free valences 'yl', 'ylidene', and 'ylidyne' in accordance with the numbering of the parent hydride. If there is a choice, the suffixes are assigned low locants, in that order. Suffixes are cited in the order 'yl', 'ylidene', and 'ylidyne'.

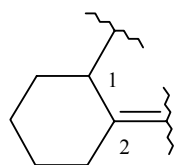
Examples:



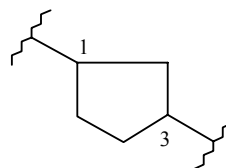
cyclohexyl (PIN)



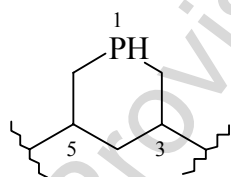
cyclopentylidene (PIN)



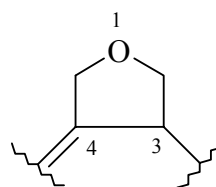
cyclohexan-1-yl-2-ylidene (PIN)



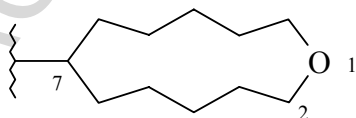
cyclopentane-1,3-diyl (PIN)



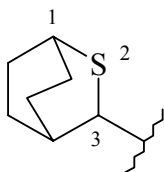
phosphinane-3,5-diyl (PIN)



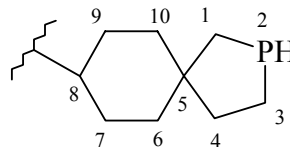
oxolane-3-yl-4-ylidene (PIN)



1-oxacyclododecan-7-yl (PIN)



2-thiabicyclo[2.2.2]octan-3-yl (PIN)

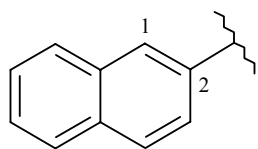


2-phosphaspiro[4.5]decan-8-yl (PIN)

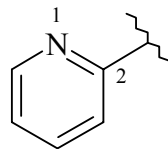
P-29.3.4 Substituent groups derived from mancude parent hydrides

P-29.3.4.1 The general method, P-29.2.2, is applied to all mancude rings and ring systems. There is no difficulty when one hydrogen atom is present to derive a monovalent substituent. When none is present or when an 'ylidene' type substituent group is needed, it is necessary to use 'added hydrogen' (see P-14.6). Formally, this method involves the adding of one hydrogen atom to the atom from which the substituent group is derived and another hydrogen atom that can be located on any atom of the ring or ring system. This 'added hydrogen atom' is expressed by the symbol *H*, preceded by a locant denoting its position.

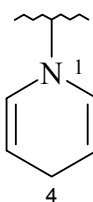
Examples:



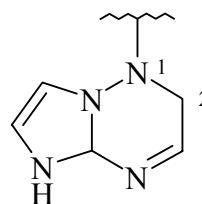
naphthalen-2-yl (PIN)



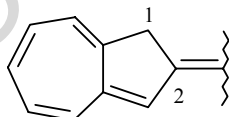
pyridin-2-yl (PIN)



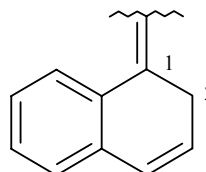
pyridin-1(4*H*)-yl (PIN)



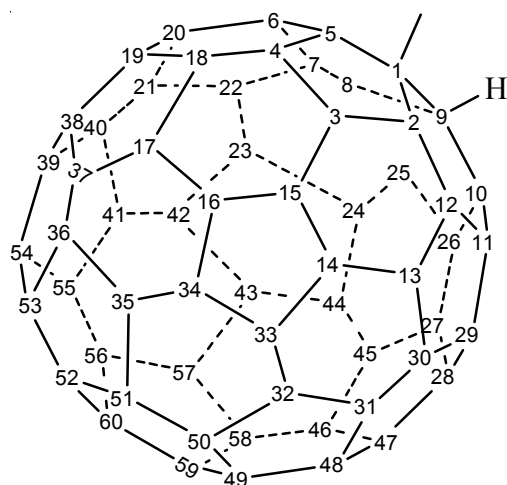
imidazo[1,2-*b*][1,2,4]triazin-1(2*H*)-yl (PIN)



azulen-2(1*H*)-ylidene (PIN)



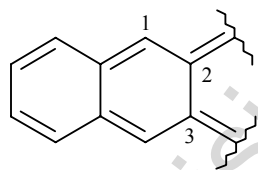
naphthalen-1(2*H*)-ylidene (PIN)



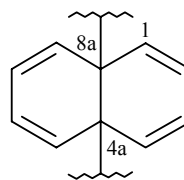
(C₆₀-I_h)[5,6]fulleren-1(9H)-yl (PIN)

P-29.3.4.2 ‘Dylydene’ substituent groups derived from mancude compounds by conversion of two –CH= groups into free valences with any necessary rearrangement of double bonds to a quinoid structure are named by adding two ‘ylidene’ suffixes, i.e. ‘dylydene’, to the parent hydride; no added hydrogen is necessary. No added hydrogen is necessary either in the case of the formation of a substituent group of the ‘diyl’ type, when the free valences are located at fusion atoms.

Examples:



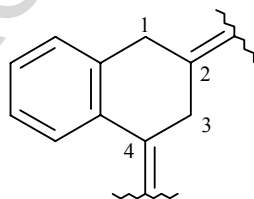
naphthalene-2,3-dylydene (PIN)



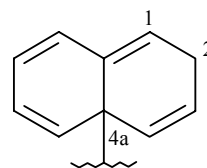
naphthalene-4a,8a-diyl (PIN)

When no quinoid structure results from the introduction of free valences, added hydrogen atoms must be cited in names. They receive the lowest possible locants. When one free valence of the ‘yl’ type is present at a fusion atom, added hydrogen must also be cited in names.

Examples:



naphthalene-2,4(1H,3H)-dylydene (PIN)



naphthalen-4a(2H)-yl (PIN)

P-29.3.5 Substituent groups derived from ring assemblies

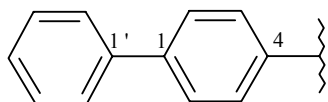
Names of substituent groups derived from ring assemblies composed of saturated rings are formed as described in Section P-28.2, and those derived from ring assemblies composed of aromatic compounds as described in P-28.3.4.1. Low locants are assigned to ring junctions, then to free valences.

Names of substituent groups derived from ring assemblies are written in two ways.

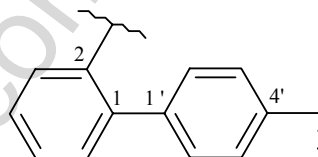
- Suffixes 'yl' and 'ylidene' are added to the name biphenyl;
- Names denoted by locants are placed in brackets; the suffixes 'yl' and 'ylidene' are added with elision of the final letter 'e' in the name of the parent hydride.

For choice of preferred IUPAC names see Chapter 5..

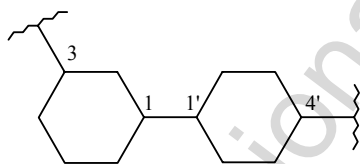
Examples:



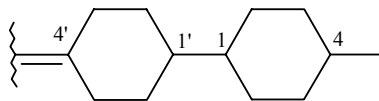
[1,1'-biphenyl]-4-yl (PIN)



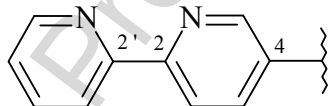
[1,1'-biphenyl]-2,4'-diyl (PIN)



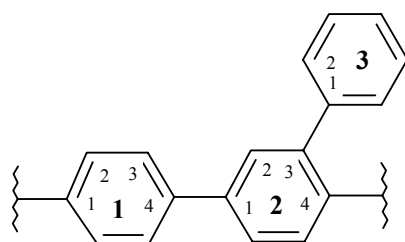
[1,1'-bicyclohexane]-3,4'-diyl (PIN)
[1,1'-bi(cyclohexyl)]-3,4'-diyl



[1,1'-bicyclohexane]-4-yl-4'-ylidene (PIN)
[1,1'-bi(cyclohexyl)]-4-yl-4'-ylidene

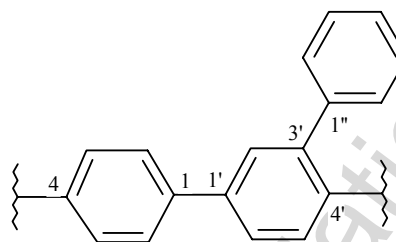


[2,2'-bipyridin]-4-yl (PIN)
[2,2'-bipyridyl]-4-yl

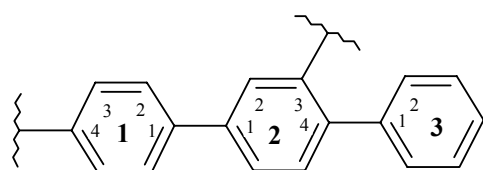


(2a) [1¹,2¹:2³,3¹-terphenyl]-1⁴,2⁴-diyl (PIN)
 (see P-28.3.1)

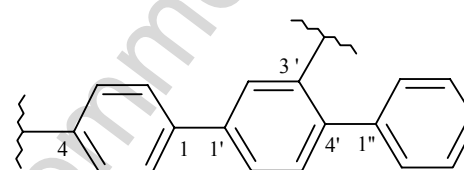
or



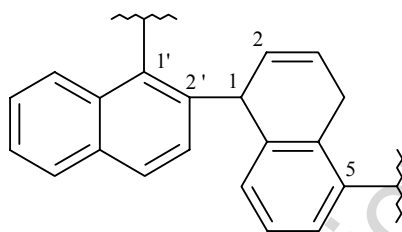
(2b) [1,1':3',1''-terphenyl]-4',4'-diyl
 (see P-28.3.1)



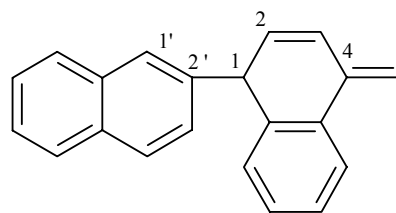
(2a) [1¹,2¹:2⁴,3¹-terphenyl]-1⁴,2³-diyl (PIN)
 (see P-28.3.1)



(2b) [1,1':4',1''-terphenyl]-3',4'-diyl
 (see P-28.3.1)



[1,2'-binaphthalene]-1',5'-diyl (PIN)
 [1,2'-binaphthyl]-1',5'-diyl

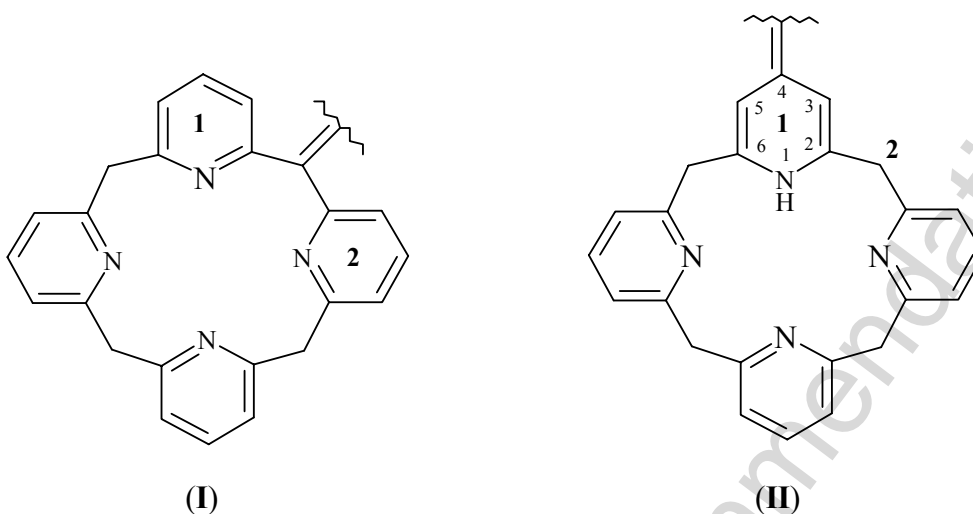


[1,2'-binaphthalen]-4(1*H*)-ylidene (PIN)
 [1,2'-binaphthyl]-4(1*H*)-ylidene

P-29.3.6 Substituent groups derived from cyclophanes

Substituent groups derived from cyclophanes are formed by applying the principles described above.

Examples:



(I) 1,5,7(2,6)-tetrapyridinacyclooctaphan-2-ylidene (PIN)
 (II) 1,3,5,7(2,6)-tetrapyridinacyclooctaphan-1⁴(1^{1H})-ylidene (PIN)

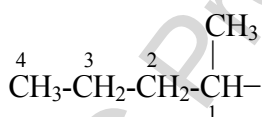
P-29.4 Compound substituent groups

A compound substituent group is formed by substituting one or more simple substituents into another simple substituent considered as the principal chain. The choice of the principal chain is fully discussed in Section P-47. The first criterion to be applied is that the principal chain is the longest chain.

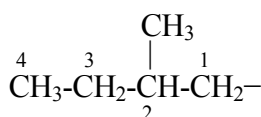
Monovalent branched substituent groups derived from homogeneous chains are named by prefixing the designation of the side chains to the name of the unbranched substituent group possessing the longest possible chain starting from the atom having the free valence, the atom with the free valence being numbered '1'. The presence of identical simple substituent groups is indicated by the appropriate multiplying prefix 'di', 'tri', 'tetra', etc.

Names of substituent groups are formed in accordance with P-29.3.

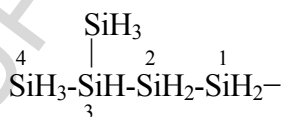
Examples:



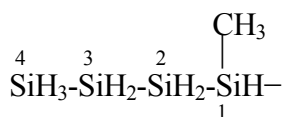
1-methylbutyl
 pentan-2-yl (PIN, see P-29.2.2)



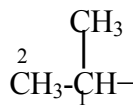
2-methylbutyl (PIN)



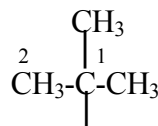
3-silyltetrasilane-1-yl (PIN)



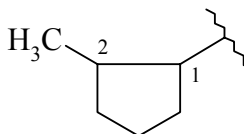
1-methyltetrasilane-1-yl (PIN)



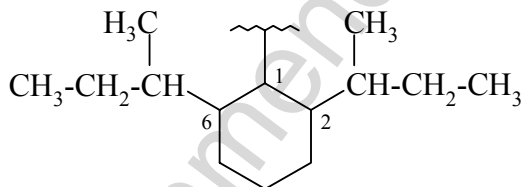
1-methylethyl
 propan-2-yl (PIN, see P-29.2.2)



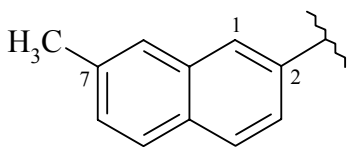
1,1-dimethylethyl (numbering shown)
 2-methylpropan-2-yl (PIN, see P-29.2.2)



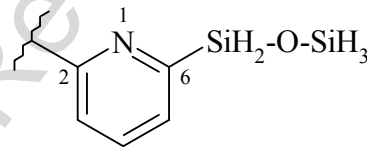
2-methylcyclopentyl (PIN)



2,6-bis(1-methylpropyl)cyclohexyl
 2,6-di(butan-2-yl)cyclohexyl (PIN)



7-methylnaphthalen-2-yl (PIN)

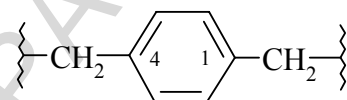
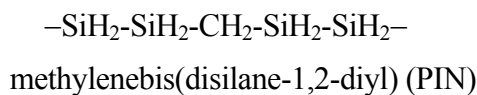
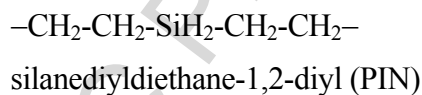


6-disiloxanylpyridin-2-yl (PIN)

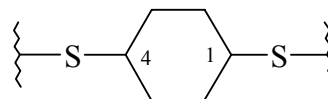
P-29.5 Compound catenated substituent groups

Compound catenated substituent groups are used only in multiplicative nomenclature (see P-15.3). Names are formed by adding di- or polyvalent substituent groups to one another, specifically by adding the names of peripheral substituent groups to that of the central substituent group, as prescribed in multiplicative nomenclature.

Examples:



1,4-phenylenebis(methylene) (PIN)
 (1,4-phenylene is a preferred
 retained IUPAC name, see P-29.6)



cyclohexane-1,4-diyylbis(sulfanediyl) (PIN)

P-29.6 Retained names for substituent groups derived from parent structures.

This Section describes retained names of substituent groups derived from parent structures. Some are IUPAC preferred names as well as names to be used in general nomenclature. The substitutability of each structure is indicated in the same manner as for the parent structures of P-34 and P-55. These types are more fully described in P-46.

Substitutability of substituent groups derived from parent structures with retained names is classified into three main types:

Type 1. Unlimited substitution by substituent groups cited as suffixes or prefixes;

Type 2. Limited substitution classified as follows:

Type 2a. Substitution limited to substituent groups cited as prefixes in recognition of functional groups explicitly expressed or implied in the functional parent compound name;

Type 2b. Substitution limited to substituent groups cited as compulsory prefixes;

Type 2c. Substitution for parent structures not covered by Type 2a or 2b.

Type 3. Substitution of any kind not allowed

Table 2.9 lists retained names for substituent groups derived from parent structures and their substitutability as defined above for use in general nomenclature and as the preferred IUPAC name, if the retained name is also the preferred IUPAC name.

To facilitate the choice of preferred IUPAC prefix names, all usual prefixes, including those described below, are listed in Appendix 2, with clear indications as to their preferred status in IUPAC nomenclature of organic compounds

In retained names, when a locant is necessary to identify a position, it is placed at the front of the name.

Table 2.10 Retained names for substituent groups derived from parent hydrides.

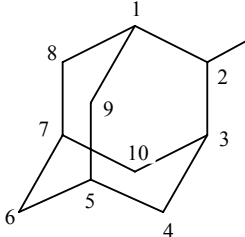
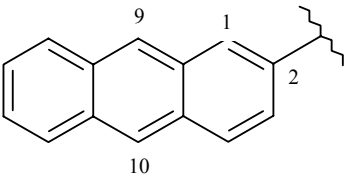
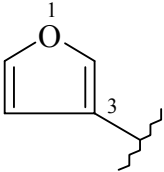
Retained Name	Structure	Substitution Type for General Nomenclature	PIN	Substitution Type for PIN
2-adamantyl (also 1-isomer)		Type 2a	adamantan-2-yl (also 1-isomer)	
2-anthryl (also 1- and 9-isomers)		Type 2a	anthracen-2-yl (also 1- and 9-isomers)	
benzyl	$C_6H_5-CH_2-$	Type 2c	benzyl	Type 3
benzylidene	$C_6H_5-CH=$	Type 2c	benzylidene	Type 3
benzylidyne	$C_6H_5-C\equiv$	Type 2a	benzylidyne	Type 3
<i>tert</i> -butyl	$(CH_3)_3C-$	Type 3	<i>tert</i> -butyl	Type 3
ethylene	$-CH_2CH_2-$	Type 2a	ethane-1,2-diyl	
3-furyl (also 2- isomer)		Type 2a	furan-3-yl (also 2- isomer)	
hydrazinyl	NH_2-NH-	Type 2a	hydrazinyl	Type 2a
isopropyl	$(CH_3)_2CH-$	Type 3	propan-2-yl	

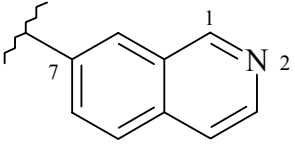
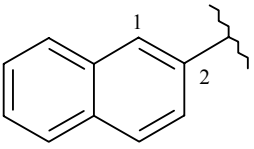
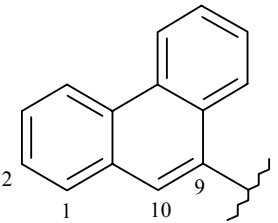
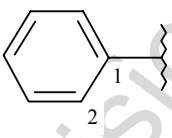
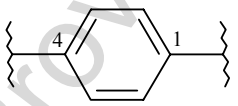
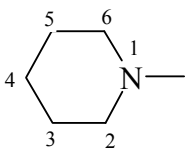
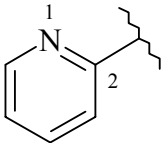
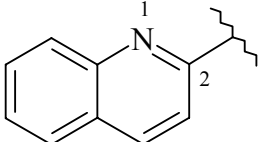
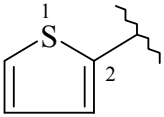
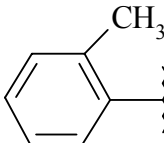
Table 2.9 (cont'd.)				
isopropylidene	$(\text{CH}_3)_2\text{C}=\text{}$	Type 3	propan-2-ylidene	
7-isoquinolyl (also 1-, 3-, 4-, 5-, 6-, and 8- isomers)		Type 2a	isoquinolin-7-yl (also 1-, 3-, 4-, 5-, 6-, and 8- isomers)	
methylene	$-\text{CH}_2-$	Type 2a	methylene	Type 2a
2-naphthyl (also 1- isomer)		Type 2a	naphthalen-2-yl (also 1- isomer)	
9-phenanthryl (also 1-, 2-, 3-, and 4- isomers)		Type 2a	phenanthren-9-yl (also 1-, 2-, 3-, and 4- isomers)	
phenyl		Type 2a	phenyl	Type 2a
1,4-phenylene (also 1,2- and 1,3-isomers) (not <i>o</i> -, <i>m</i> -, or <i>p</i> -isomers)		Type 2a	1,4-phenylene (also 1,2- and 1,3- isomers) (not <i>o</i> -, <i>m</i> -, or <i>p</i> - isomers)	Type 2a
1-piperidyl (not piperidino) (also 2-,3-,and 4-isomers)		Type 2a	piperidin-1-yl (also 2-, 3-, and 4- isomers)	

Table 2.9 (cont'd.)			
2-pyridyl (also 3- and 4- isomers)		Type 2a	pyridin-2-yl (also 3- and 4- isomers)
2-quinolyl (also 3-, 4-, 5-, 6-, 7-, and 8- isomers)		Type 2a	quinolin-2-yl (also 3-, 4-, 5-, 6-, 7-, and 8- isomers)
styryl	$C_6H_5-CH=CH-$	Type 3	2-phenylethenyl
2-thienyl (also 3- isomer)		Type 2a	thiophen-2-yl (also 3- isomer) (CAS uses thiophene-2-yl)
<i>o</i> -tolyl (also <i>m</i> - and <i>p</i> - isomers)		Type 3	2-methylphenyl (also 3- and 4- isomers)
trityl	$(C_6H_5)_3C-$	Type 3	triphenylmethyl