

CHAPTER P-2 PARENT HYDRIDES

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P-20 Introduction

A parent hydride is the structure that is named before the addition of affixes denoting substituents to yield the name of a specific compound. Its name is understood to signify a definite population of hydrogen atoms attached to a skeletal structure. Acyclic parent hydrides are always saturated and unbranched, for example, pentane and trisilane. Cyclic parent hydrides are usually either fully saturated, for example, cyclopentane, cyclotrisiloxane, azepane, bicyclo[3.2.1]octane, and spiro[4.5]decane, or fully unsaturated, i.e., they contain the maximum number of noncumulative double bonds, for example, benzene, pyridine, 1,3-oxazole, 1*H*-phenalene, phenanthroline and benzo[*a*]acridine. Also, there are parent hydrides that are partially saturated, for example, spiro[1,3-dioxolane-2,1'-[1*H*]indene], and there are combinations of cyclic and acyclic hydrides, having traditional retained names, for example toluene.

Names of parent hydride names that do not contain skeletal carbon atoms, for example trisilane, are not designated as preferred IUPAC names in these recommendations. Instead they are called preselected, i.e., they are used to generate preferred IUPAC for derivatives substituted by organic (carbon-containing) substituents (see P-12.2). They may, however, become IUPAC preferred names depending on decisions of a team formed to decide IUPAC preferred names for inorganic (noncarbon-containing) compounds.

Names of parent hydrides are either traditional names that are retained or systematic names formed in accordance with specific rules. Rules and names must be unambiguous and clear. In order to achieve this goal and keep rules simple and concise, the rules for selecting preferred IUPAC names and preselected names of parent hydrides and prefixes denoting substituent groups derived from parent hydrides are not provided in this Chapter. These rules are given in Chapter 5.

P-21 Mononuclear and acyclic polynuclear parent hydrides

- P-21.1 Mononuclear parent hydrides
- P-21.2 Acyclic polynuclear parent hydrides

P-21.1 Mononuclear parent hydrides

P-21.1.1 Mononuclear hydrides with standard bonding numbers

P-21.1.1.1 Systematic names

The names of mononuclear hydrides of the elements for use as parents in naming organic compounds by substitutive nomenclature are given in Table 2.1. Most are formed systematically by combining the 'a' term of the element (with elision of the terminal letter 'a' before the ending 'ane', patterned after methane, for example, borane for BH_3 , silane for SiH_4 , etc.). There are important exceptions: methane, which is the retained name for CH_4 , oxidane for H_2O , sulfane for H_2S , selane for H_2Se , tellane for H_2Te , polonane for H_2Po , and bismuthane for BiH_3 (see Table 2.1). The systematically formed names oxane, thiane, selenane, tellurane, polane, and bismane, are Hantzsch-Widman names designating the corresponding saturated six-membered rings with a single heteroatom. 'Carbane' has never been used in place of methane; it is not recommended.

Table 2.1 Systematic names of mononuclear hydrides of Groups 13, 14, 15, 16 and 17 with normal bonding numbers
 (all names except for methane are preselected)

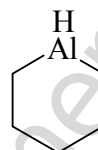
Groups	13	14	15	16	17
	BH_3	CH_4	NH_3	OH_2	FH
	borane	methane	azane	oxidane	fluorane
	AlH_3	SiH_4	PH_3	SH_2	ClH
	alumane	silane	phosphane	sulfane	chlorane
	InH_3	GeH_4	AsH_3	SeH_2	BrH
	indigane	germane	arsane	selane	bromane
	GaH_3	SnH_4	SbH_3	TeH_2	IH
	gallane	stannane	stibane	tellane	iodane
	TlH_3	PbH_4	BiH_3	PoH_2	HAt
	thallane	plumbane	bismuthane	polane	astatane

The newly recommended names gallane and thallane are formed systematically. Alumane and indigane are exceptions. The name 'aluminane' could be ambiguous as it could designate the mononuclear hydride AlH_3 and the saturated six-membered ring with one aluminium atom that has a Hantzsch-Widman name denoted by the ending '-inane'. The name 'alane' has been used, but must also be discarded because its systematically derived substituent group, $\text{H}_2\text{Al}-$, would be named 'alanyl', the well entrenched name for the acyl group derived from the amino acid alanine. The name

alumane has no negative connotation. The prefix 'aluma' is recommended for forming Hantzsch-Widman names, and thus, the name 'aluminane' describes the saturated six-membered ring monocycle containing one aluminium atom (see P-22.2.2). The systematically formed name 'indane' cannot be used because it is already used to designate a partially saturated bicyclic fused hydrocarbon. Reich and Richter (ref. 15) called the element indium in 1863 after the indigo colored flame test, recognized as different than the color from caesium. Returning to the source indigo, 'indigane' could be an acceptable name; it is thus recommended for the hydride InH_3 .



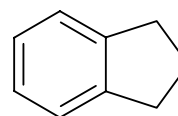
alumane (preselected name; see P-12.2)
(not alane)



aluminane (PIN)



indigane (preselected name; see P-12.2)



indane
2,3-dihydro-1*H*-indene (PIN)

The monohydride names listed in Table 2.1 constitute the basis of 'generalized ane nomenclature'. Substitutive nomenclature as applied to alkanes, cycloalkanes and polycycloalkanes has been systematically extended to hydrides of elements of Groups 13, 14, 15, 16, and 17. Generalized 'ane' nomenclature is divided into 'carbane nomenclature', which covers the traditional substitutive nomenclature for carbon parent hydrides, and 'heterane nomenclature', which relates to atoms other than carbon, the 'heteroatoms' in the nomenclature of organic compounds.

P-21.1.1.2 Retained names

The names 'phosphine', PH_3 , 'arsine', AsH_3 , 'stibine', SbH_3 , and 'bismuthine', BiH_3 , are not retained.

The common names water, ammonia, the binary names for the hydracids of Group 17, for example hydrogen chloride, and binary names for the hydrides of Group 16, for example hydrogen sulfide, are retained. However, systematic alternatives to these common names, e.g. oxidane for water and azane for ammonia; and for the binary names of hydracids of Group 17 and the hydrides of Group 16, e.g., chlorane for hydrogen chloride and sulfane for hydrogen sulfide, are necessary for naming some derivatives and for generating names of radicals, ions, and polynuclear homologues.

P-21.1.2 Mononuclear parent hydrides with nonstandard bonding numbers

P-21.1.2.1 Systematic names

If the bonding number of the element differs from the standard one as defined in P-14.1 and exemplified in Table 2.1, the name of the hydride is modified by affixing the symbol λ^n , where 'n' is the bonding number, to the name of the hydride (see P-14.1).

P-21.1.2.2 Retained names

The names 'phosphorane', PH_5 ; 'arsorane', AsH_5 ; 'stiborane', SbH_5 ; are retained for use in general nomenclature. However, the names 'sulfurane', H_4S ; 'selenurane', H_4Se ; 'iodinane', H_3I ; 'persulfurane', H_6S ; and 'periodinane', H_5I , which have been used in recent literature, are not recommended.

Examples:

H_3I λ^3 -iodane (preselected name; see P-12.2) (not iodinane)	H_4S λ^4 -sulfane (preselected name; see P-12.2) (not sulfurane)
SnH_2 λ^2 -stannane (preselected name: see P-12.2)	PH_5 λ^5 -phosphane (preselected name; see P-12.2) phosphorane
AsH_5 λ^5 -arsane (preselected name; see P-12.2) arsorane	SbH_5 λ^5 -stibane (preselected name; see P-12.2) stiborane

P-21.2 Acyclic polynuclear parent hydrides

P-21.2.1 Hydrocarbons

P-21.2.2 Homogeneous acyclic parent hydrides other than hydrocarbons and boron hydrides

P-21.2.3 Heterogenous acyclic parent hydrides

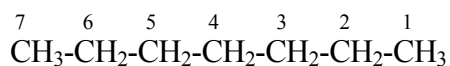
P-21.2.4 Acyclic parent hydrides containing heteroatoms with nonstandard bonding numbers

P-21.2.1 Hydrocarbons

The saturated unbranched acyclic hydrocarbons C_2H_6 , C_3H_8 , and C_4H_{10} have the retained names ethane, propane, and butane, respectively. Systematic names for the higher members of this series consist of a numerical term (see Table 1.4), followed by the ending 'ane' with elision of the terminal letter 'a' from the numerical term. The generic name for saturated acyclic hydrocarbons (branched or

unbranched) is 'alkane'. The chain is numbered from one end to the other with arabic numbers. Brackets are employed in formulas to indicate repetition of groups in chains.

Examples:



heptane (PIN)



icosane (PIN)
(the Beilstein and CAS index
name is 'eicosane')



tricosane (PIN)

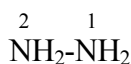


heptacontane (PIN)

P-21.2.2 Homogeneous acyclic parent hydrides other than hydrocarbons and boron hydrides

A compound consisting of an unbranched chain containing two or more identical heteroatoms saturated with hydrogen atoms is named by citing the appropriate multiplying prefix from Table 1.4 (with no elision of the terminal vowel of the multiplying prefix) followed by the name of the appropriate hydride according to P-2.1. These names are preselected (see P-12.2).

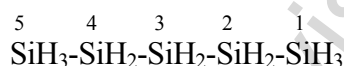
Examples:



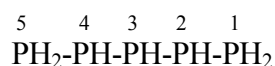
hydrazine (retained name, preselected; see P-12.2)
diazane



nonaazane (preselected name; see P-12.2)



pentasilane (preselected name; see P-12.2)



pentaphosphane (preselected name; see P-12.2)

P-21.2.3 Heterogeneous acyclic parent hydrides. There are two types to be considered.

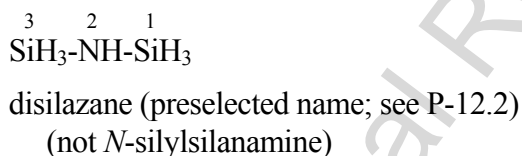
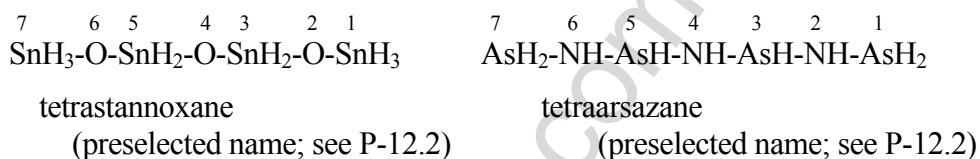
P-21.2.3.1 Heterogeneous parent hydrides composed of alternating atoms

P-21.2.3.2 Heterogeneous parent hydrides formed by skeletal replacement ('a')
nomenclature

P-21.2.3.1 Heterogeneous parent hydrides composed of alternating heteroatoms, i.e., [a(ba)_n hydrides], excluding carbon atoms

Compounds containing an unbranched chain of alternating atoms terminated by two identical atoms of the element coming later in the seniority order F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn < Pb > B > Al > Ga > In > Tl may be named by citing successively a multiplying prefix denoting the number of atoms of the terminal element followed by the 'a' term for that element, then the 'a' term of the other element in the chain and the ending 'ane'. The terminal letter 'a' of an 'a' term is elided when followed by a vowel; the terminal vowel of a numerical prefix is not elided even when the 'a' term begins with the same vowel. When nitrogen atoms are present, names of amines could be considered as alternative names but are not recommended. These parent hydrides have priority to receive preferred names, as long as they are used to name carbon containing compounds, i.e., they are preselected names.

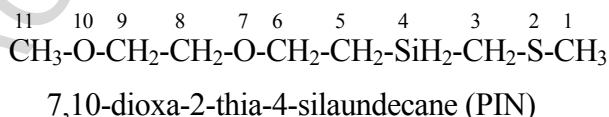
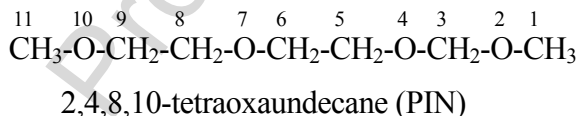
Examples:



P-21.2.3.2 Heterogeneous parent hydrides formed by skeletal replacement ('a') nomenclature

Heterogeneous acyclic parent hydrides consisting of chains containing at least one carbon atom and at least four heteroatoms, alike or different, and terminating with C, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, or Tl are named by skeletal replacement ('a') nomenclature (see P-15.4.2.1).

Examples:



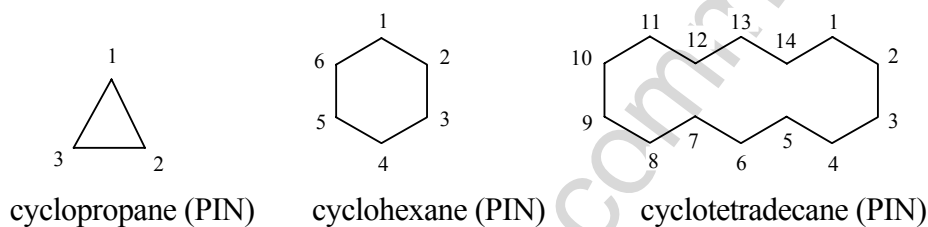
P-22 Monocyclic parent hydrides

- P-22.1 Monocyclic hydrocarbons
- P-22.2 Heteromonocyclic parent hydrides

P-22.1 Monocyclic hydrocarbons

P-22.1.1 The names of saturated monocyclic hydrocarbons are formed by attaching the nondetachable prefix 'cyclo' to the name of the acyclic saturated unbranched hydrocarbon with the same number of carbon atoms. The generic name of monocyclic hydrocarbons is 'cycloalkane'. Numbering proceeds sequentially around the ring.

Examples:

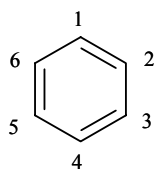


P-22.1.2 Unsubstituted monocyclic hydrocarbon polyenes having the maximum number of non-cumulative double bonds and with the general formula of C_nH_n or C_nH_{2n+1} , (with n greater than 6) are called annulenes generically. A specific annulene is named as an $[n]$ annulene, where n is the number of carbon atoms of the ring and is greater than 6. When n is an odd number, i. e., when the annulene has the general formula C_nH_{2n+1} , the extra hydrogen atom is denoted as 'indicated hydrogen' (see P-14.6) and is assigned the locant '1'. Such annulene names may be used in general nomenclature and are the IUPAC preferred names for parent components in fusion nomenclature. Preferred IUPAC names for fully unsaturated monocyclic hydrocarbons are those of the corresponding cycloalkapolyenes (see P-31.1.3.1).

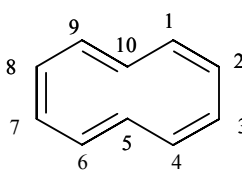
Benzene is the retained name for C_6H_6 ; the name $[6]$ annulene is not recommended. Annulene names are used as parent components in fusion nomenclature (see P-25.3.2.1.1); but are not used as component prefixes.

In the numbering of annulenes, the locant '1' is placed at any carbon atom in structures having an even number of carbon atoms; in annulenes having an odd number of carbon atoms, the locant '1' is assigned to the carbon atom bearing the indicated hydrogen (see P-14.6). In cycloalkapolyene structures, the locant '1' is always assigned to a carbon atom of a double bond.

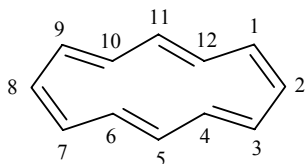
Examples:



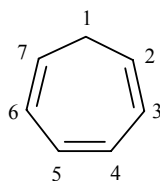
benzene (PIN)
(not [6]annulene)



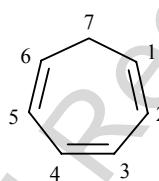
[10]annulene
cyclodeca-1,3,5,7,9-pentaene (PIN)



[12]annulene
cyclododeca-1,3,5,7,9,11-hexaene (PIN)

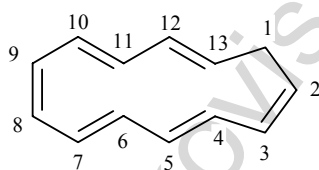


(I)

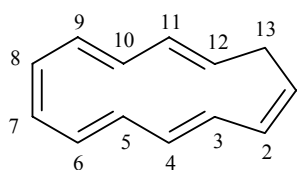


(II)

(I) 1*H*-[7]annulene
(II) cyclohepta-1,3,5-triene (PIN)



(I)

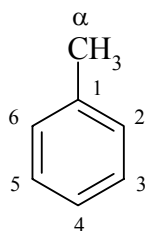


(II)

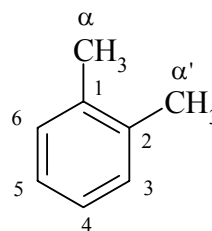
(I) 1*H*-[13]annulene
(II) cyclotrideca-1,3,5,7,9,11-hexaene (PIN)

P-22.1.3 Parent structures having retained names

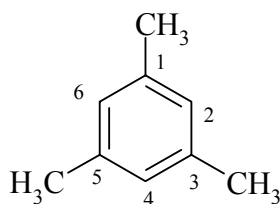
Toluene, xylene and mesitylene are specific parent hydrides that are composed of two components, one cyclic and the other acyclic and saturated. These names are retained due to a long and well established tradition. Toluene and xylene are preferred IUPAC names, but are not substitutable; toluene is substitutable under certain conditions (see P-46.3) for general nomenclature. Mesitylene is a retained name in general nomenclature only and cannot be substituted.



toluene (PIN)
(see P-46.3.1 for substitution rules)



xylene (1,2-, 1,3-, and 1,4-isomers, PINs)
(no substitution)
o-, *m*-, and *p*-xylene



mesitylene
1,3,5-trimethylbenzene (PIN)

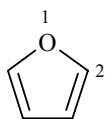
P-22.2 Heteromonocyclic parent hydrides

- P-22.2.1 Retained names and derived names of chalcogen analogues
- P-22.2.2 Monocycles with 3-10 membered rings (Hantzsch-Widman names)
- P-22.2.3 Heteromonocyclic hydrides named by skeletal replacement ('a') nomenclature
- P-22.2.4 Homogeneous monocyclic hydrides other than hydrocarbons and boron hydrides
- P-22.2.5 Heteromonocyclic hydrides composed of repeating units
- P-22.2.6 Heteromonocyclic hydrides having heteroatoms with nonstandard bonding numbers

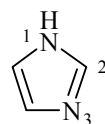
P-22.2.1 Retained names and names of derived chalcogen analogues

The retained names are listed in Table 2.2. The name 'pyran' can be modified by functional replacement to generate names for chalcogen analogues.

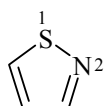
Table 2.2 Retained names of mancude heteromonocyclic parent hydrides



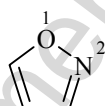
furan (PIN)



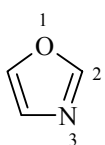
imidazole (PIN)
(1*H* isomer shown)



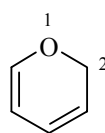
isothiazole
1,2-thiazole (PIN)



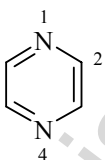
isoxazole
1,2-oxazole (PIN)



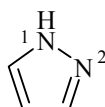
oxazole
1,3-oxazole (PIN)



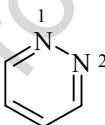
pyran (2*H*-isomer shown) (PIN)
thiopyran (S instead of O) (PIN)
selenopyran (Se instead of O) (PIN)
telluropyan (Te instead of O) (PIN)



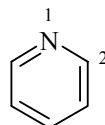
pyrazine (PIN)



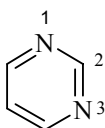
pyrazole (PIN)
(1*H*-isomer shown)



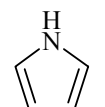
pyridazine (PIN)



pyridine (PIN)

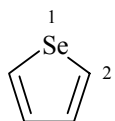


pyrimidine (PIN)

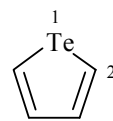


pyrrole (PIN)
(1*H*-isomer shown)

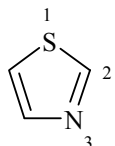
Table 2.2 (cont'd)



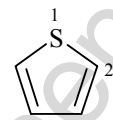
selenophene (PIN)



tellurophene (PIN)

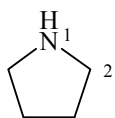


thiazole
1,3-thiazole (PIN)

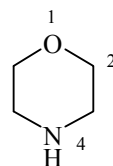


thiophene (PIN)

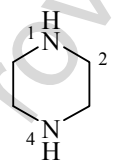
Table 2.3 Retained names of saturated heteromonocyclic parent hydrides used as preferred names and in general nomenclature



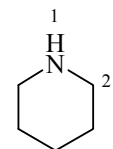
pyrrolidine (PIN)



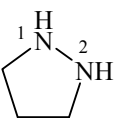
morpholine (PIN)
thiomorpholine (S instead of O) (PIN)
selenomorpholine (Se instead of O) (PIN)
telluromorpholine (Te instead of O) (PIN)



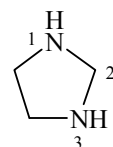
piperazine (PIN)



piperidine (PIN)



pyrazolidine (PIN)



imidazolidine (PIN)

P-22.2.2 Monocycles with 3-10 membered rings (Hantzsch-Widman names)

Monocyclic compounds with no more than ten ring members and containing one or more heteroatoms are named by using the extended Hantzsch-Widman system (ref. 15). Homogeneous heteromonocycles are preselected (see P-12.2).

The elements aluminium, gallium, indium, and thallium are now included in the recommended Hantzsch-Widman system and mercury has been deleted.

P-22.2.2.1 Constructing and numbering Hantzsch-Widman names

P-22.2.2.1.1 Hantzsch-Widman names are formed by combining the 'a' prefix(es) for the heteroatom(s) (Table 2.4) with a stem indicating the size of the ring and the degree of hydrogenation (Table 2.5). Vowels between 'a' prefixes and between the 'a' prefix and the stem are elided. Unsaturated compounds are those having the maximum number of noncumulative double bonds (monocyclic compounds) and at least one double bond. The presence of a single heteroatom determines the numbering in a monocyclic compound; the heteroatom has the locant '1'.

Hantzsch-Widman names are preferred IUPAC names for both the unsaturated and saturated compounds. Hantzsch-Widman names are preselected names for homogeneous heteromonocycles other than hydrocarbons (see P-22.2.5).

Table 2.4 Hantzsch-Widman system prefixes (in decreasing order of seniority)

Element	Bonding number (Valence)	Prefix	Element	Bonding number (Valence)	Prefix
fluorine	1	fluora	antimony	3	stiba
chlorine	1	chlora	bismuth	3	bisma
bromine	1	broma	silicon	4	sila
iodine	1	ioda	germanium	4	germa
oxygen	2	oxa	tin	4	stanna
sulfur	2	thia	lead	4	plumba
selenium	2	selena	boron	3	bora
tellurium	2	tellura	aluminium	3	aluma ¹ (not alumina)
nitrogen	3	aza	gallium	3	galla
phosphorus	3	phospha	indium	3	indiga ¹ (not inda)

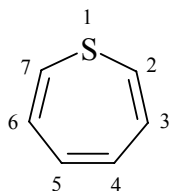
arsenic 3 arsa thallium 3 thalla

¹ Compare with Table 1.5

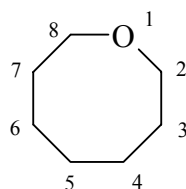
Table 2.5 Hantzsch-Widman system stems

Ring Size	Unsaturated	Saturated	Ring Size	Unsaturated	Saturated
3	irene/irine	irane/iridine	7	epine	epane
4	ete	etane/etidine	8	ocine	ocane
5	ole	olane/olidine	9	onine	onane
6A	ine	ane	10	ecine	ecane
6B (N, Si, Ge, Sn, Pb)	ine	inane			
6C (F, Cl, Br, I, N, P, As Sb, Al, Ga, In, Tl)	inine	inane			

Examples:



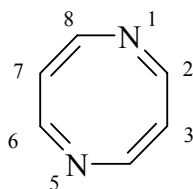
thiepine (PIN)



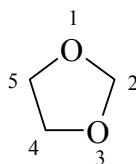
oxocane (PIN)

P-22.2.2.1.2 A multiplicity of the same heteroatom is indicated by a multiplying prefix 'di', 'tri', 'tetra', etc., placed before the appropriate 'a' term. The final letter of a multiplying prefix is not elided before a vowel. Lowest possible locants are assigned to heteroatoms, locant '1' being assigned to one of the heteroatoms. Locants are cited at the front of the name, i.e., before the 'a' term and any preceding numerical prefixes.

Examples:



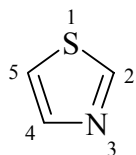
1,5-diazocine (PIN)



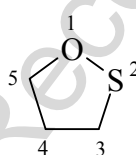
1,3-dioxolane (PIN)

P-22.2.2.1.3 If two or more kinds of heteroatoms occur in the same name, their order of citation follows the sequence: F, Cl, Br, I, O, S, Se, Te, N, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, Tl, Hg. The locant '1' is given to a heteroatom that occurs first in the seniority sequence used for citation of the 'a' prefixes. The numbering is then chosen to give lowest locants to heteroatoms considered as a set in ascending numerical order. Locants are cited at the front of the name, in the order of citation of the 'a' prefixes.

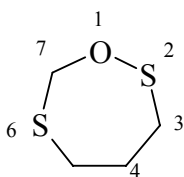
Examples:



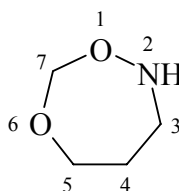
1,3-thiazole (PIN)



1,2-oxathiolane (PIN)



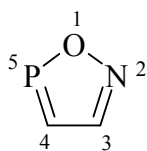
1,2,6-oxadithiepane (PIN)
(not 1,3,7-oxadithiepane;
the locant set '1,2,6' is
lower than '1,3,7')



1,6,2-dioxazepane (PIN)
(not 1,3,4-dioxazepane; not
1,3,7-dioxazepane; not 1,6,5-
dioxazepane; the locant set
'1,2,6' is lower than '1,3,4';
'1,3,7'; or '1,5,6')

If there is a further choice, lowest locants are assigned to heteroatoms in the order that they appear in the seniority sequence (see Table 2.3).

Example:

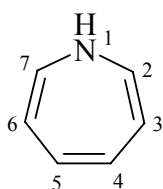


1,2,5-oxazaphosphole (PIN)
(not 1,5,2-oxazaphosphole; N has
priority over P for lowest locant)

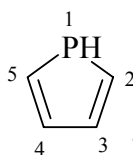
P-22.2.2.1.4 Indicated hydrogen

After the maximum number of noncumulative double bonds has been assigned, any ring atom with a bonding order of three or higher connected to adjacent ring atoms by single bonds only, and carrying one or more hydrogen atoms, is designated by the indicated hydrogen symbol *H*. If there is a choice, such ring atoms are selected for low locants.

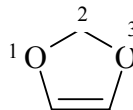
Examples:



1*H*-azepine (PIN)



1*H*-phosphole (PIN)



2*H*-1,3-dioxole (PIN)

P-22.2.2.1.5 Selecting Hantzsch-Widman names for 3-, 4-, or 5-membered rings

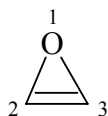
As shown in Table 2.4, for monocyclic three-membered rings and saturated three-, four-, and five-membered rings two stems are recommended. They are used as follows:

- (a) The stem 'irine' is used in place of 'irene' for rings containing only nitrogen; otherwise the stem 'irene' is used.

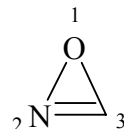
Examples:



1*H*-azirine (PIN)



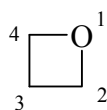
oxirene (PIN)



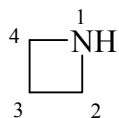
oxazirine (PIN)

- (b) The stems 'iridine', 'etidine' and 'olidine' are used when nitrogen atoms are present in the ring; otherwise the 'ane' stems are used.

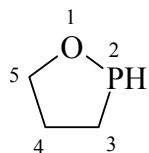
Examples:



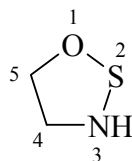
oxetane (PIN)



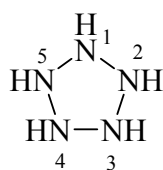
azetidine (PIN)



1,2-oxaphospholane (PIN)



1,2,3-oxathiazolidine (PIN)

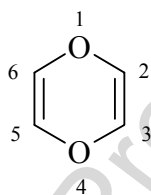


pentaazolidine (preselected name; see P-12.2)

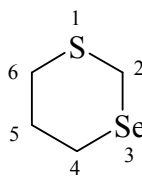
P-22.2.2.1.6 Selecting Hantzsch-Widman names for six-membered rings

The stem for six-membered rings depends on the least senior heteroatom in the ring, i.e., the heteroatom whose name directly precedes the ending. Heteroatoms are divided into three groups, A, B, and C, each corresponding to a stem for the unsaturated and for the saturated compound (Table 2.5). The stem is selected in accordance with the group to which the **least** senior heteroatom belongs.

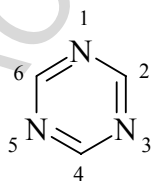
Examples:



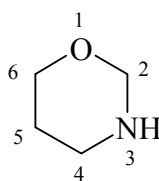
1,4-dioxine (PIN)



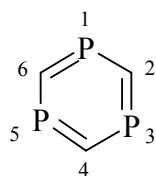
1,3-thiaselenane (PIN)



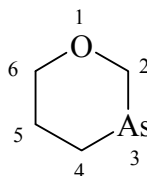
1,3,5-triazine (PIN)



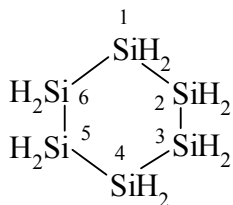
1,3-oxazinane (PIN)



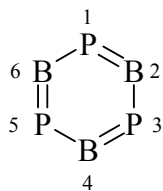
1,3,5-triphosphinine (PIN)



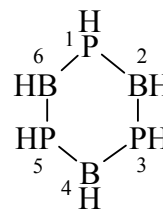
1,3-oxarsinane (PIN)



hexasilinane (preselected name; see P-12.2)



1,3,5,2,4,6-triphosphatriborinine
(preselected name; see P-12.2)



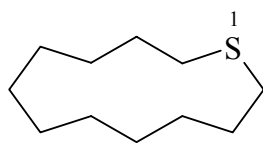
1,3,5,2,4,6-triphosphatriborinane
(preselected name; see P-12.2)

P-22.2.3 Heteromonocyclic hydrides named by skeletal replacement ('a') nomenclature

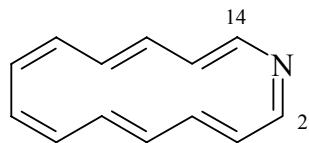
Mancude and saturated heteromonocyclic compounds with up to and including ten ring members are named by the extended Hantzsch-Widman system. For monocyclic rings with eleven and more ring members, skeletal replacement ('a') nomenclature is used for the fully saturated or fully unsaturated compounds ([*n*]annulenes).

P-22.2.3.1 Skeletal replacement names are formed by placing 'a' prefixes in front of the name of the corresponding cycloalkane or annulene, and, when more than one heteroatom is present, in the following decreasing seniority order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl. For numbering, see P-22.2.3.2.

Examples:



thiacyclododecane (PIN)

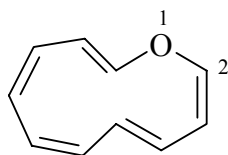


1-azacyclotetradeca-1,3,5,7,9,11,13-heptaene (PIN)
aza[14]annulene

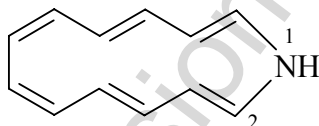
P-22.2.3.2 Numbering

P-22.2.3.2.1 When a single heteroatom is present in the ring, it is assigned the locant '1', which is omitted in the name, unless a locant for an indicated hydrogen atom is present. Low locants are assigned first to the heteroatom and then to unsaturated sites (see P-31.1.3.2). When required, locants for indicated hydrogen atoms are assigned in accordance with P-14.6.

Examples:



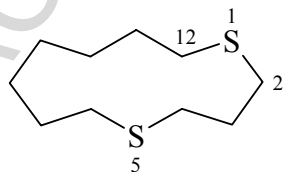
1-oxacycloundeca-2,4,6,8,10-pentaene (PIN)
oxa[11]annulene



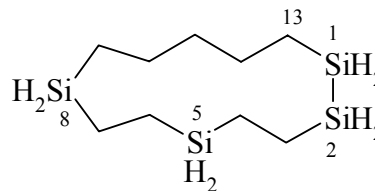
1H-1-azacyclotrideca-2,4,6,8,10,12-hexaene (PIN)
1H-1-aza[13]annulene

P-22.2.3.2.2 When the same kind of heteroatom occurs more than once, the direction of numbering is chosen to give the lower locants to the heteroatoms as a set.

Examples:



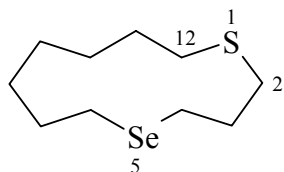
1,5-dithiacyclododecane (PIN)



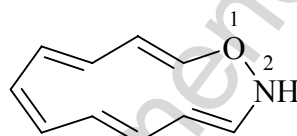
1,2,5,8-tetrasilacyclotridecane (PIN)

P-22.2.3.2.3 When heteroatoms of different kinds are present, the locant '1' is given to the heteroatom first cited in the order of seniority given above (see P-22.2.3.1). The direction of numbering is then chosen to give lower locants to the heteroatoms as a set without regard to the kind of heteroatom, and then, if necessary, according to the order of seniority above (see P-22.2.3.1). Low locants are assigned first to the heteroatoms and then to the unsaturated sites (see P-31.1.3.2). When required, locants for indicated hydrogen atoms are assigned in accordance with P-14.6.

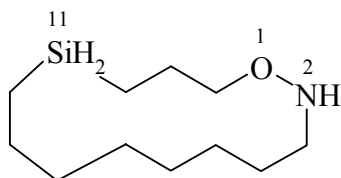
Examples:



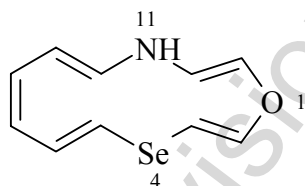
1-thia-5-selenacyclododecane (PIN)



1-oxa-2-azadodeca-3,5,7,9,11-pentanene (PIN)
2H-1-oxa-2-aza[12]annulene



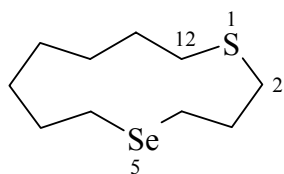
1-oxa-2-aza-11-silacyclotetradecane (PIN)



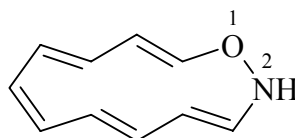
1-oxa-4-selena-11-azatrideca-2,5,7,9,12-pentaene (PIN)
1H-1-oxa-4-selena-11-aza[13]annulene

P-22.2.3.2.3 When heteroatoms of different kinds are present, the locant '1' is given to the heteroatom first cited in the order of seniority given above (see P-22.2.3.1). The direction of numbering is then chosen to give lower locants to the heteroatoms as a set without regard to the kind of heteroatom, and then, if necessary, according to the order of seniority above (see P-22.2.3.1). Low locants are assigned first to the heteroatoms and then to the unsaturated sites (see P-31.1.3.2). When required, locants for indicated hydrogen atoms are assigned in accordance with P-14.6.

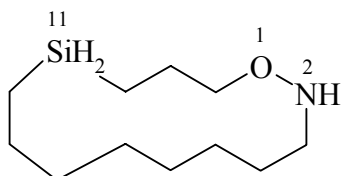
Examples:



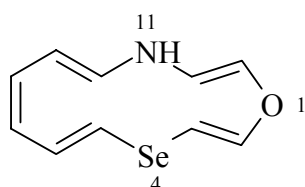
1-thia-5-selenacyclododecane (PIN)



1-oxa-2-aza-cyclododeca-3,5,7,9,11-pentaene (PIN)
2*H*-1-oxa-2-aza[12]annulene



1-oxa-2-aza-11-silacyclotetradecane (PIN)



1-oxa-4-selena-11-azacyclotrideca-2,5,7,9,12-pentaene (PIN)
11*H*-1-oxa-4-selena-11-aza[13]annulene

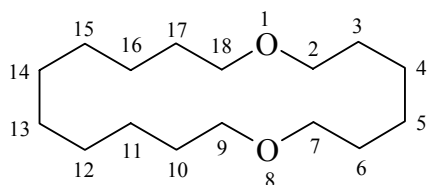
P-22.2.4 Heteromonocycles with eleven or more members having the maximum number of noncumulative double bonds (for generating component names in fusion nomenclature).

Names of heteromonocyclic parent components with more than ten ring members for use in fusion nomenclature are discussed in this subsection. They are used to generate names of components for preferred IUPAC names of fused ring systems; they have also been used as names for the heteromonocycle in general nomenclature as an alternative to the cycloalkapolyene names that are preferred IUPAC names for the heteromonocycles.

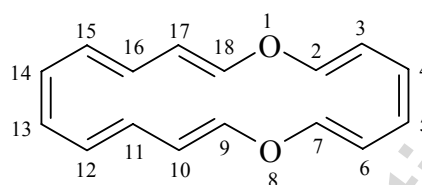
A heteromonocyclic parent component having more than ten members and the maximum number of noncumulative double bonds (mancude) is named by changing the ending 'ane' of the name corresponding to the saturated heteromonocycle (see P- 22.2.3) to 'ine'. Indicated hydrogen atoms are designated as required.

For examples of fusion compounds including this type of heteromonocyclic component, see P-25.2.2.4, P-25.3.6.1 and P-25.3.7.1.

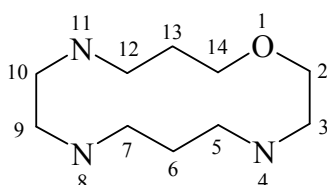
Examples:



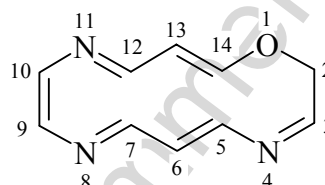
1,8-dioxacyclooctadecane (PIN)



1,8-dioxacyclooctadecene
 1,8-dioxacyclooctadeca-2,4,6,9,11,13,15,17-
 octaene (PIN)



1-oxa-4,8,11-triazacyclotetradecane (PIN)

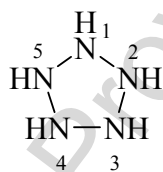


2*H*-1-oxa-4,8,11-triazacyclotetradecene
 1-oxa-4,8,11-triazacyclotetradeca-3,5,7,9,11,13-
 hexaene (PIN)

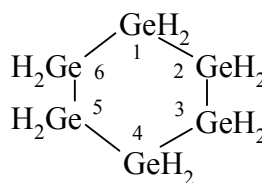
P-22.2.5 Homogeneous monocyclic hydrides other than hydrocarbons and boron hydrides

A saturated heteromonocycle consisting of identical heteroatoms can be named by adding the prefix 'cyclo' to the name of the saturated rectilinear chain that has the same number of identical atoms. For alternative methods, see the Hantzsch-Widman extended system described in P-22.2.2 for 3 to 10 membered rings and skeletal replacement ('a') nomenclature described in P-22.2.3. The names used to generate preferred IUPAC names for organic derivatives of these heteromonocyclic hydrides are preselected (see P-12.2).

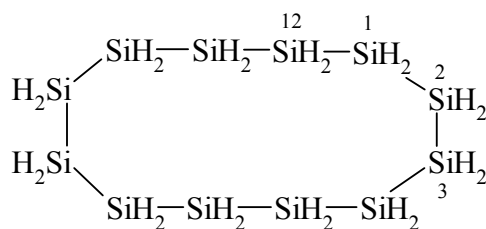
Examples:



cyclopentaaazane
 pentazolane
 (preselected name; see P-12.2)



cyclohexagermane
 hexagerminane
 (preselected name; see P-12.2)

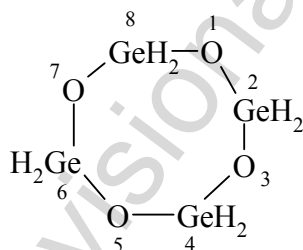


cyclododecasilane
dodecasilacyclododecane (preselected name; see P-12.2)

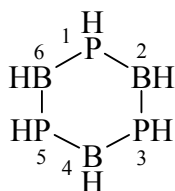
P-22.2.6 Heteromonocyclic hydrides composed of repeating units [(ab)_n cyclic hydrides]

Names may be constructed by citing successively the prefix ‘cyclo’, a multiplying affix (‘di’, ‘tri’, ‘tetra’, etc.) indicating the number of each element in the ring, the ‘a’ terms for the atoms of the repeated unit first cited in the order Tl > In > Ga > Al > Pb > Sn > Ge > Si > Bi > Sb > As > P > N > Te > Se > S > O, and the ending ‘ane’. The terminal letter of an ‘a’ term is elided when followed by a vowel; the terminal letter of a multiplying affix is not elided even when the ‘a’ term begins with a vowel. Numbering starts at one of the skeletal atoms of the element cited last in the name and proceeds continuously around the ring. For alternative methods, see P-22.2.2 for Hantzsch-Widman names and P-22.2.3 for naming monocycles with more than ten members. The names used to generate preferred IUPAC names for organic derivatives of these heteromonocyclic hydrides are preselected (see P-12.2).

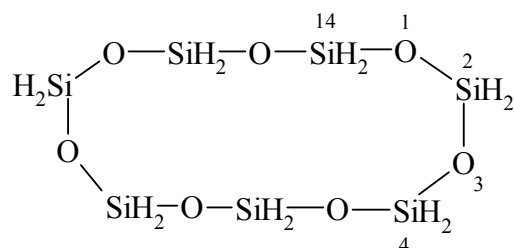
Examples:



cyclotetragermoxane
1,3,5,7,2,4,6,8-tetraoxatetragermocane (preselected name, see P-12.2)



cyclotriboraphosphane
1,3,5,2,4,6-triphosphatriborinane (preselected name, see P-12.2)

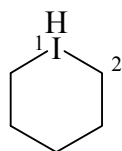


cycloheptasiloxane (see P-22.2.5)
 1,3,5,7,9,11,13-hepta-oxa-2,4,6,8,10,12,14-heptasilacyclotetradecane
 (preselected name, see P-12.2)

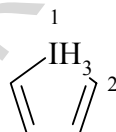
P-22.27 Heteromonocyclic hydrides having heteroatoms with nonstandard bonding numbers.

P-22.2.7.1 The λ -convention is used to denote heteroatoms with nonstandard bonding numbers in heteromonocycles (see P-14.1). The symbol λ^n , where n is the bonding number, is cited immediately after the locant denoting the heteroatom with the nonstandard bonding number. The symbol H , if required to denote saturated skeletal atoms, is cited at the front of the complete name with the appropriate locant(s).

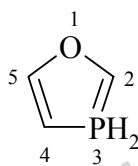
Examples:



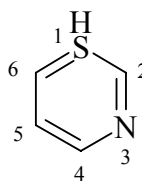
1 λ^3 -iodinane (PIN)



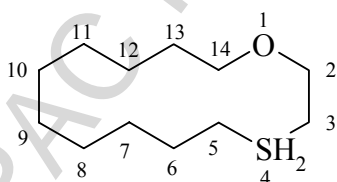
1 H -1 λ^5 -iodole (PIN)



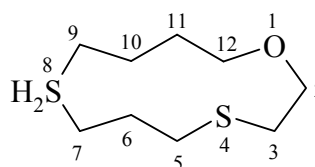
1,3 λ^5 -oxaphosphole (PIN)



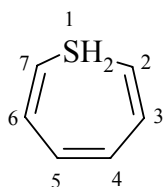
1 λ^4 ,3-thiazine (PIN)



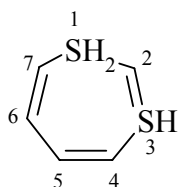
1-oxa-4 λ^4 -thiacyclotetradecane (PIN)



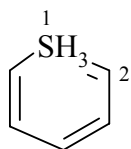
1-oxa-4,8 λ^4 -dithiacyclododecane (PIN)



1H-1 λ^4 -thiepine (PIN)



1H-1 λ^4 ,3 λ^4 -dithiepine (PIN)
[the (–SH₂–) group, which includes an indicated hydrogen, is preferred for the low locant]

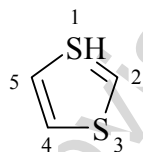


1 λ^6 -thiopyran (PIN)

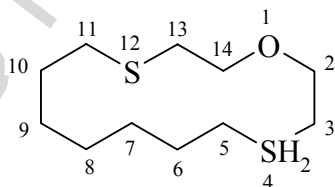
(this heteromonocycle has the maximum number of double bonds and one double bond at every position; hence, no indicated hydrogen is cited for the sulfur atom)

P-22.2.7.2 If a further choice is needed between two or more of the same skeletal atom with different bonding numbers, the lower locant is assigned in order of the decreasing value of the bonding number, i.e., λ^6 is selected over λ^4 (see also P-21.2.4).

Examples:



1 λ^4 ,3-dithiole (PIN)



1-oxa-4 λ^4 ,12-dithiacyclotetradecane (PIN)

P-23 Extended von Baeyer system for polycyclic compounds

- P-23.0 Introduction
- P-23.1 Definitions and terminology
- P-23.2 Naming and numbering von Baeyer hydrocarbons
- P-23.3 Heterogeneous heterocyclic von Baeyer parent hydrides
- P-23.4 Homogeneous heterocyclic von Baeyer parent hydrides
- P-23.5 Heterogeneous heterocyclic von Baeyer parent hydrides composed of alternating heteroatoms
- P-23.6 Heterocyclic polycyclic parent hydrides having heteroatoms with nonstandard bonding numbers
- P-23.7 Retained names for von Baeyer parent hydrides

P-23.0 Introduction

This section is based on the recent publication 'Extension and Revision of the von Baeyer system for naming polycyclic compounds (including bicyclic compounds) (IUPAC Recommendations 1999) (ref. 7). It supersedes Rules A-31, A-32 and B-14 in the 1979 Recommendations (ref. 1) and Rule R-2.4.2 in the 1993 Recommendations (ref. 2). No modifications to the 1999 publication have been made in this Section.

This Section deals only with saturated polycyclic ring systems named by the von Baeyer system; for unsaturated systems, see Section P-31.1.4. For naming substituent groups derived from saturated polycyclic ring systems, see Section P-29.

P-23.1 Definitions and terminology

P-23.1.1 A 'bridgehead' is any skeletal atom of the ring system that is bonded to three or more skeletal atoms (excluding hydrogen).

P-23.1.2 A 'bridge' is an unbranched chain of atoms or an atom or a valence bond connecting two bridgeheads.

P-23.1.3 The 'main ring' is the ring system that includes as many skeletal atoms of the polycyclic system as possible.

P-23.1.4 The 'main bridge' is the bridge included in a bicyclic system and the first selected bridge in a polycyclic system.

P-23.1.5 Two bridgeheads are selected as 'main bridgeheads'. These two bridgeheads are included in the main ring and connected by the main bridge.

P-23.1.6 A 'secondary bridge' is any bridge not included in the main ring or the main bridge.

P-23.1.7 An 'independent secondary bridge' links bridgeheads which are part of the main ring or main bridge.

P-23.1.8 A 'dependent secondary bridge' links at least one bridgehead that is part of a secondary bridge.

P-23.1.9 A 'polycyclic system' contains a number of rings equal to the minimum number of scissions required to convert the system into an acyclic skeleton. The number of rings is indicated by the non-detachable prefix, 'bicyclo' (not dicyclo), 'tricyclo', 'tetracyclo', etc.

P-23.2 Naming and numbering von Baeyer hydrocarbons

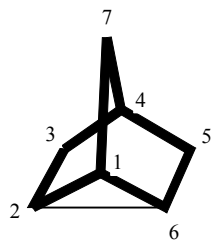
Bi- and polycyclic hydrocarbons that are treated by the von Baeyer system are named by the following rules applied in order until a decision is reached.

- P-23.2.1 Selection of the main ring
- P-23.2.2 Naming of bicyclic alicyclic hydrocarbons
- P-23.2.3 Numbering of bicyclic alicyclic hydrocarbons
- P-23.2.4 Selection of the main bridge
- P-23.2.5 Naming and numbering of tricyclic alicyclic hydrocarbons
- P-23.2.6 Naming and numbering of polyalicyclic hydrocarbons

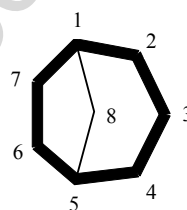
P-23.2.1 Selection of the main ring

The main ring of a polycyclic hydrocarbon ring system is selected so as to include as many skeletal atoms of the structure as possible. The main ring is shown in bold in subsections P-23.2.1 through P-23.2.6.

Examples:



a six membered main ring



a seven membered main ring

P-23.2.2 Naming bicyclic alicyclic hydrocarbons

Saturated homogeneous bicyclic hydrocarbons having two or more atoms in common are named by prefixing 'bicyclo' to the name of the acyclic hydrocarbon having the same total number of skeletal atoms. The numbers of skeletal atoms in each of the two segments connecting the main bridgeheads and in the main bridge are given by arabic numbers cited in descending numerical order separated by full stops and enclosed in square brackets.

Example:

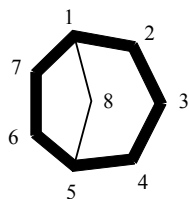


bicyclo[3.2.1]octane (PIN)

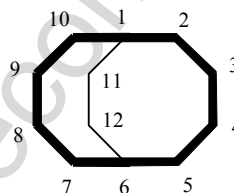
P-23.2.3 Numbering bicyclic alicyclic hydrocarbons

The bicyclic ring system is numbered starting with one of the bridgeheads and proceeding first along the longer segment of the main ring to the second bridgehead, then back to the first bridgehead along the unnumbered segment of the main ring. Numbering is completed by numbering the main bridge beginning with the atom next to the first bridgehead.

Examples:



bicyclo[3.2.1]octane (PIN)

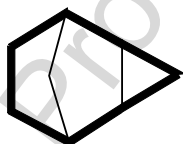


bicyclo[4.4.2]dodecane (PIN)

P-23.2.4 Selection of the main bridge

In a polycyclic ring system there is more than one bridge connecting atoms of the main ring and/or the main bridge. The main bridge (like the main ring shown herein in bold) is the one that includes as many of the atoms not included in the main ring as possible. Bridges other than the main bridge are called 'secondary bridges'.

Example:



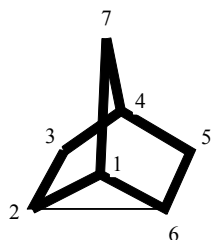
P-23.2.5 Naming and numbering tricyclic alicyclic hydrocarbons

P-23.2.5.1 Tricyclic hydrocarbons having an independent secondary bridge are named on the basis of a bicyclic system described in P-23.2.2. Rings not described by the bicyclic system are defined by citing the number of atoms in the independent secondary bridge as an arabic number. The locants of the two attachment points of the independent secondary bridge to the main ring are cited as a pair of superscript arabic numbers (lower first) separated by a comma.

The name of the tricyclic system is then constructed by citing:

- the prefix 'tricyclo', in place of 'bicyclo', indicating the presence of three rings in the polycyclic system;
- numbers indicating the bridge lengths (with the appropriate superscript locants for the secondary bridge) separated by full stops and placed in brackets (e.g. [2.2.1.0^{2,5}]);
- the name of the acyclic hydrocarbon having the same total number of skeletal atoms.

Examples:



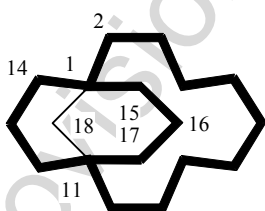
tricyclo[2.2.1.0^{2,6}]heptane (PIN)

P-23.2.5.2 Numbering the secondary bridge

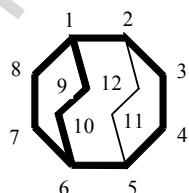
After the main ring and main bridge have been numbered, the independent secondary bridge is numbered continuing from the higher numbered bridgehead of the main ring.

This Rule and Rule P-23.2.6.3 replace Rule A-32.23 in the 1979 Recommendations (ref. 1) and Rule R-2.4.2.2 in the 1993 Recommendations (ref. 2).

Examples:



tricyclo[9.3.3.1^{1,11}]octadecane (PIN)



tricyclo[4.2.2.2^{2,5}]dodecane (PIN)
(the secondary bridge is numbered
starting from bridgehead 5)

P-23.2.6 Naming and numbering polycyclic alicyclic hydrocarbons

Polycyclic analogues of saturated bi- and tricyclic ring systems (P-23.2.3 and P-23.2.5) are named as described in the following subsections. Independent and dependent secondary bridges are considered here. Rules for numbering all secondary bridges and for naming all polyalicyclic systems are described; their application follows those described for naming and numbering bicyclic systems as described in P-23.2.1 to P-23.2.4 above. An additional rule is necessary to select the main bridge and the secondary bridges.

P-23.2.6.1 Naming polycyclic alicyclic hydrocarbons

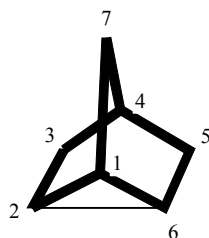
Rings not designated by the bicyclic system described above (P-23.2.2) are defined by citing the number of atoms in each secondary bridge as an arabic number. The locants of the two attachment points of each secondary bridge to the main ring are cited as a pair of superscript arabic numbers (lower first) separated by a comma. The numbers indicating independent secondary bridges (bridges that connect atoms of the bicyclic system) are cited in decreasing order. The procedure for construction of names is given in the following subsections.

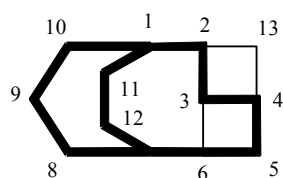
P-23.2.6.1.1 The prefixes 'tricyclo', 'tetracyclo', etc., in place of 'bicyclo', indicate the number of rings in the polyalicyclic system. The number of rings is equal to the number of bond cuts necessary to transform the polycyclic system into an acyclic unbranched or branched skeleton.

P-23.2.6.1.2 The number of atoms in each bridge additional to the main bridge, i.e., the secondary bridges, is indicated by arabic numbers separated by full stops and cited in decreasing numerical order following those describing the bicyclic system, except as provided by P-23.6.1.3. The location of each secondary bridge is indicated by the arabic number locants of the bicyclic structure already numbered; these locants are cited as superscripts to the arabic number denoting its length (number of atoms) and separated by a comma. The assemblage of arabic numbers denoting the length of bridges with superscript numbers, if necessary, is commonly called the 'von Baeyer descriptor'; it is enclosed in brackets.

P-23.2.6.1.3 Independent secondary bridges are cited before dependent secondary bridges. The numbers indicating dependent secondary bridges are cited in decreasing order (the third example in P-23.2.6.3 illustrates this order of citation).

P-23.2.6.1.4 The name is terminated by the name of the alkane representing the total number of ring atoms; this number corresponds to the sum of the arabic numbers in the numerical descriptor enclosed by brackets plus two (for the two main bridgehead atoms); for example, in the name for the following structure, bicyclo[2.2.1.0^{2,6}]heptane, the total number of ring atoms, 7, equals the sum $[2 + 2 + 1 + 0] + 2$

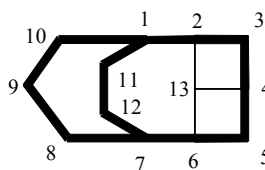




tetracyclo[5.3.2.1^{2,4}.0^{3,6}]tridecane (PIN)

correct

not



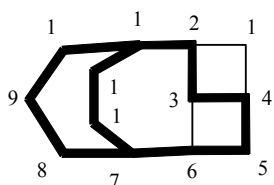
tetracyclo[5.3.2.1^{2,4}.0^{6,13}]tridecane

incorrect

(there are no dependent bridges in the correct structure; there is one dependent bridge in the incorrect structure, between 6 and 13)

P-23.2.6.2.4 The superscript locants for the secondary bridges must be as low as possible when considered as a set in ascending numerical order, the decision being made at the first point of difference.

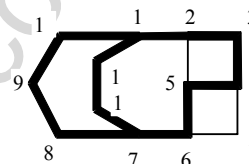
Examples:



tetracyclo[5.3.2.1^{2,4}.0^{3,6}]tridecane (PIN)

correct

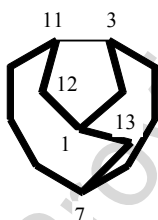
not



tetracyclo[5.3.2.1^{4,6}.0^{2,5}]tridecane

incorrect

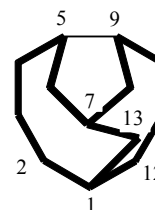
(the locant set '2,3,4,6' is lower than '2,4,5,6')



tricyclo[5.5.1.0^{3,11}]tridecane (PIN)

correct

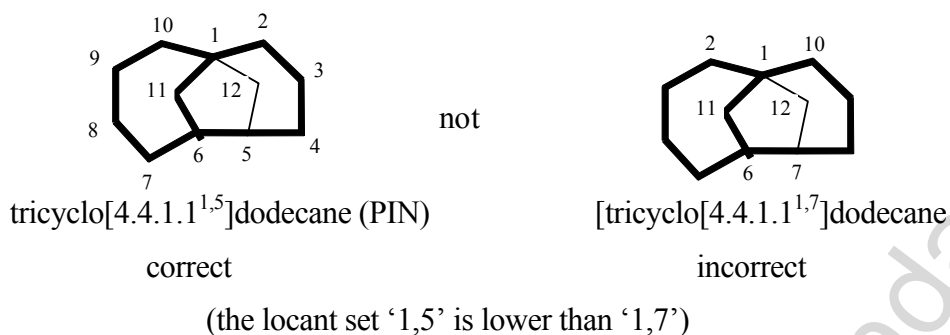
not



tricyclo[5.5.1.0^{5,9}]tridecane

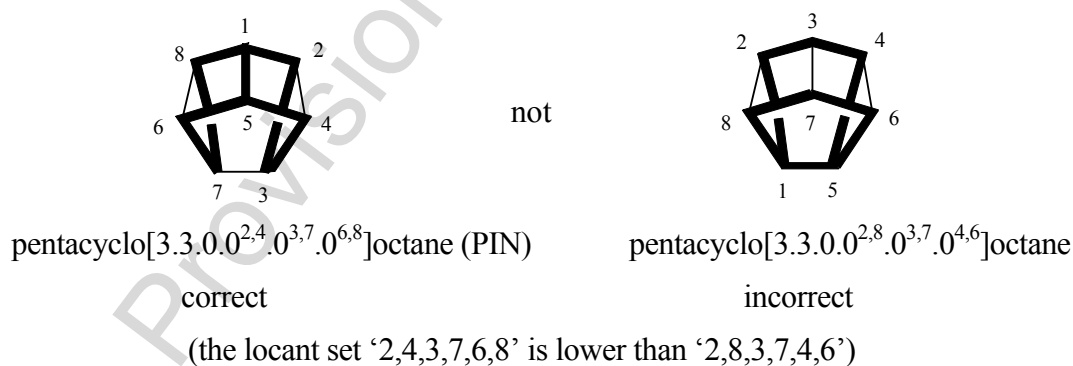
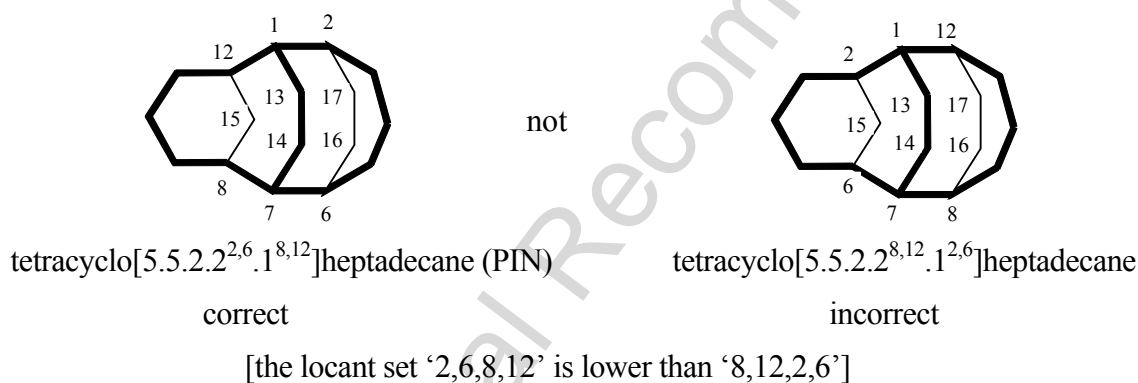
incorrect

(the locant set '3,11' is lower than '5,9')



P-23.2.6.2.5 The superscript locants shall be as low as possible when considered in their order of citation in the name.

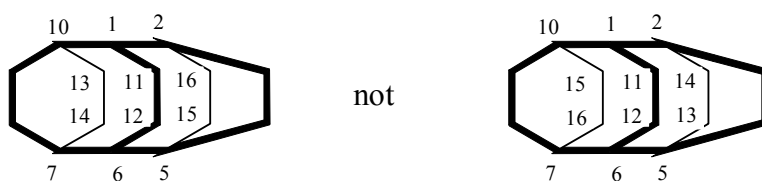
Example:



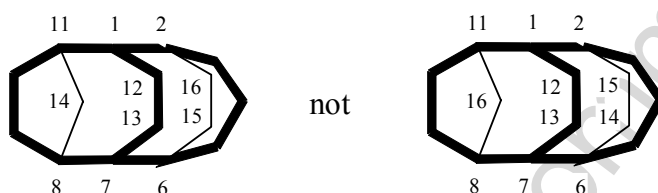
P-23.2.6.3 Numbering of secondary bridges

After numbering the main ring and main bridge, independent secondary bridges are numbered before dependent secondary bridges; the numbering continues from the highest number of the main ring and main bridge. Each secondary bridge is numbered in turn starting with the independent secondary bridge linked to the highest numbered bridgehead atom, then the independent secondary bridge linked to the next highest bridgehead atom, and so on. Each atom of a secondary bridge is numbered starting with the atom next to the higher numbered bridgehead.

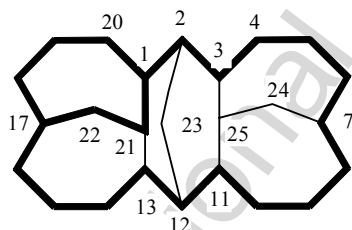
Examples:



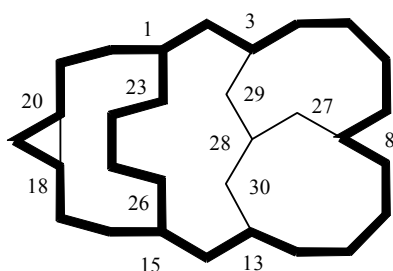
tetracyclo[4.4.2.2^{2,5}.2^{7,10}]hexadecane (PIN)
 (the first secondary bridge to be numbered
 is linked to bridgehead 10)



tetracyclo[5.4.2.2^{2,6}.1^{8,11}]hexadecane (PIN)
 (the first secondary bridge to be numbered
 is linked to bridgehead 11)

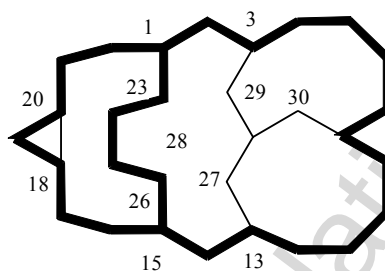


hexacyclo[15.3.2.2^{3,7}.1^{2,12}.0^{13,21}.0^{11,25}]pentacosane (PIN)
 (the dependent secondary bridge between atoms numbered 11 and 25 is cited last;
 in the numeric descriptor, the numbers '15, 3, and 2' describe the basic bicyclic
 system; the numbers '2^{3,7}, 1^{2,12}, and 0^{13,21}' correspond to the three independent
 secondary bridges; the number '0^{11,25}' corresponds to the dependent secondary
 bridge)



pentacyclo[13.7.4.3^{3,8}.0^{18,20}.1^{13,28}]triacontane (PIN)
 pentacyclo[13.7.4.3^{3,13}.0^{18,20}.1^{8,28}]triacontane

correct



not

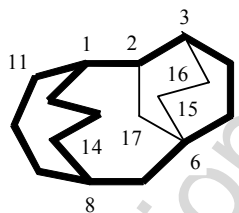
incorrect

(the independent bridge is numbered before the dependent bridge; the locant set '3,8,18,20,13,28' is lower than '3,13,18,20,8,28')

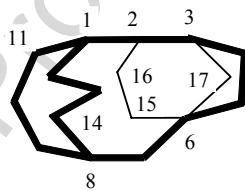
P-23.2.6.4 If there is a further choice for numbering the secondary bridges, the following criteria are considered in order until a decision can be made.

P-23.2.6.4.1 Lower locants are used for the atoms of the bridge linked to the higher numbered bridgehead.

Examples:



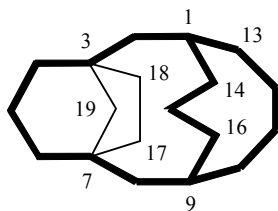
tetracyclo[6.3.3.2^{3,6}.1^{2,6}]heptadecane (PIN)
 (locants 15 and 16 are assigned to the bridge linked to bridgehead atom 3 not 2)



tetracyclo[6.3.3.2^{2,6}.1^{3,6}]heptadecane (PIN)
 (the locant 15 is assigned to the bridge linked to bridgehead atom 3 not 2)

P-23.2.6.4.2 Longer bridges are numbered before shorter bridges.

Example:



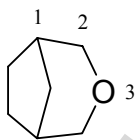
tetracyclo[7.4.3.2^{3,7}.1^{3,7}]nonadecane (PIN)

(the two atom bridge between bridgehead atoms 3 and 7 is numbered before the one atom bridge between the same two bridgehead atoms.)

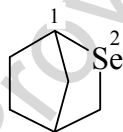
P-23.3 Heterogeneous heterocyclic von Baeyer parent hydrides

P-23.3.1 The only general method to name heterogeneous heterocyclic von Baeyer systems is skeletal replacement ('a') nomenclature. The 'a' prefixes denoting the heteroatoms are placed in front of the name of the corresponding hydrocarbon named according to P-23.2, cited in the order F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl. Numbering is determined first by the fixed numbering of the hydrocarbon system.

Examples:



3-oxabicyclo[3.2.1]octane (PIN)

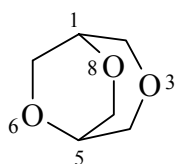


2-selenabicyclo[2.2.1]heptane (PIN)

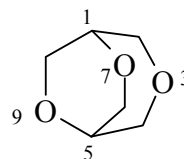
P-23.3.2 When there is a choice for numbering, the following criteria are applied in order until a decision can be made.

P-23.3.2.1 Low locants are assigned to the heteroatoms considered together as a set compared in increasing numerical order. The preferred numbering is the lowest set at the first point of difference.

Example:



not



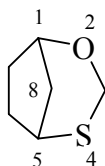
3,6,8-trioxabicyclo[3.2.2]nonane (PIN)

[3,7,9-trioxabicyclo[3.2.2]nonane

[the locant set '3,6,8' is lower than '3,7,9']

P-23.3.2.2 If there is still a choice, low locants are assigned in accord with the decreasing seniority order of heteroatoms: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Example:



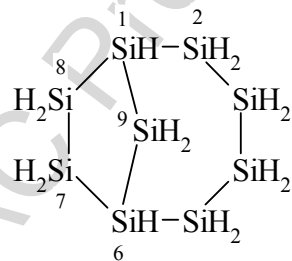
2-oxa-4-thiabicyclo[3.2.1]octane (PIN)

P-23.4 Homogeneous heterocyclic von Baeyer parent hydrides

Heterocyclic von Baeyer systems composed entirely of the same heteroatom are named:

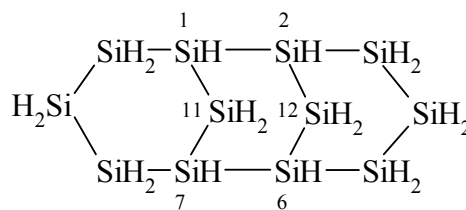
- as described for bi- and polycyclic hydrocarbons in P-23.2 and P-24 using the name of the acyclic parent hydride that has the same total number of skeletal atoms; or
- by skeletal replacement nomenclature using the 'a' prefixes described in P-23.2, in which the total number of heteroatoms is indicated by a numerical term. In either method it is not necessary to give the location of the heteroatoms because all positions are modified by the same heteroatom. Method (a) gives preselected names.

Examples:



(a) bicyclo[4.2.1]nonasilane
 (preselected name; see P-12.2)

(b) nonasilabicyclo[4.2.1]nonane



(a) tricyclo[5.3.1.1^{2,6}]dodecasilane
 (preselected name; see P-12.2)

(b) dodecasilatricyclo[5.3.1.1^{2,6}]dodecane

P-23.5 Heterogeneous heterocyclic systems composed of alternating hetero atoms

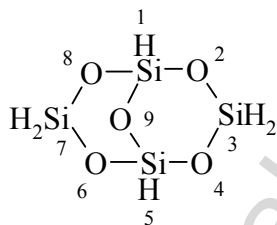
P-23.5.1 Heterogeneous von Baeyer systems composed of alternating skeletal heteroatoms may be named in two ways:

- (a) by citing a nondetachable prefix ‘bicyclo’, ‘tricyclo’, etc. before a von Baeyer descriptor (see P-23.2.6.1.2) enclosed in square brackets and then, successively:
 - (i) a multiplying prefix, ‘di’, ‘tri’, etc., denoting the number of heteroatoms that are first cited as ‘a’ terms;
 - (ii) the ‘a’ terms denoting the heteroatoms of the system in the reverse order of the recommended seniority for ‘a’ prefixes (for example, Si before O; see P-23.3.1);
 - (iii) the ending ‘ane’.

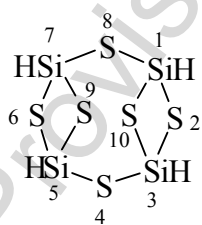
Numbering is the same as for the corresponding hydrocarbon (see P-23.1.3 and 23.1.6);

- (b) by applying normal skeletal replacement (‘a’) nomenclature to the corresponding hydrocarbon.

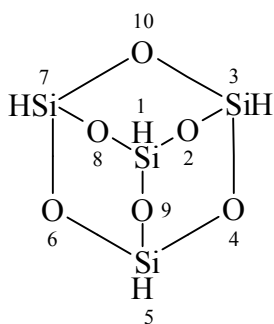
Examples:



- (a) bicyclo[3.3.1]tetrasiloxane
- (b) 2,4,6,8,9-pentaoxa-1,3,5,7-tetrasilabicyclo[3.3.1]nonane
(preselected name; see P-12.2)



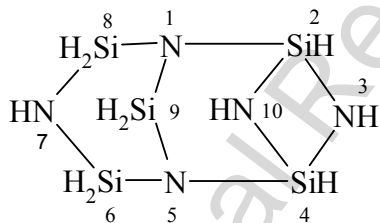
- (a) tricyclo[5.1.1.1^{3,5}]tetrasilathiane
- (b) 2,4,6,8,9,10-hexathia-1,3,5,7-tetrasilabicyclo[5.1.1.1^{3,5}]decane
(preselected name; see P-12.2)



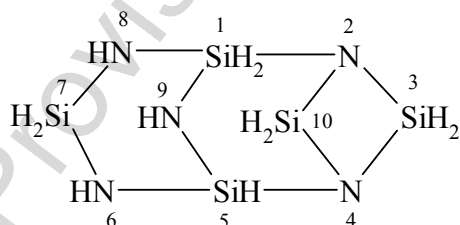
- (a) tricyclo[3.3.1.1^{3,7}]tetrasiloxane
 (b) 2,4,6,8,9,10-hexaoxa-1,3,5,7-tetrasilabicyclo[3.3.1.1^{3,7}]decane
 (preselected name; see P-12.2)

P-23.5.2 Prefixes such as '*ISi-*' or '*IN-*' are used when it is necessary to indicate the atom at the bridgehead that is to have the locant '1'. Names are identified as (a) and (b) according to the two methods described in P-23.5.1.

Example:



- (a) *IN*-tricyclo[3.3.1.1^{2,4}]pentasilazane
 (b) 1,3,5,7,10-pentaaza-2,4,6,8,9-pentasilatricyclo[3.3.1.1^{2,4}]decane
 (preselected name; see P-12.2)



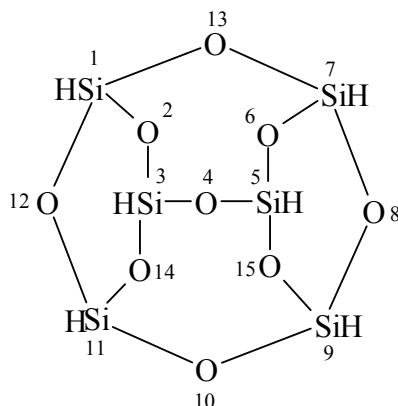
- (a) *1Si*-tricyclo[3.3.1.1^{2,4}]pentasilazane
 (b) 2,4,6,8,9-pentaaza-1,3,5,7,10-pentasilatricyclo[3.1.1.1^{2,4}]decane
 (preselected name; see P-12.2)

P-23.5.3 Silasesquioxanes, silasesquithianes, etc.

Compounds in which each silicon atom is linked to three oxygen atoms and in which every atom of oxygen is linked to two silicon atoms are named generically silasesquioxanes. Similarly, when the oxygen atoms are replaced by S, Se, Te, or N atoms, the compounds are generically called

silasesquithianes, silasesquiazanes, and so forth. They are named by the method described in P-23.5.1(a). The silasesquioxanes have the general formula $\text{Si}_{2n}\text{H}_{2n}\text{O}_{3n}$. The names tetrasilasesquioxanes ($n = 2$), hexasilasesquioxanes ($n = 3$), etc., are class names indicating $\text{Si}_{2n}\text{H}_{2n}\text{E}_{3n}$ where $\text{E} = \text{O}, \text{S}, \text{Se}, \text{Te}$ or N . The silasesquiazanes have the general formula $\text{Si}_{2n}\text{H}_{3n}\text{N}_{3n}$.

Example:

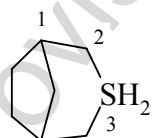


tetracyclo[5.5.1.1^{3,11}.1^{5,9}]hexasiloxane (a hexasilasesquioxane)
 2,4,6,8,10,12,13,14,15-nonaoxa-1,3,5,7,9,11-hexasilatetracyclo[5.5.1.1^{3,11}.1^{5,9}]-
 pentadecane (preselected name; see P-12.2)

P-23.6 Heterocyclic polyalicyclic parent hydrides having heteroatoms with nonstandard bonding numbers

P-23.6.1 The λ -convention, characterized by the symbol λ^n , where ' n ' is the bonding number of the heteroatom, is used to identify heteroatoms with nonstandard bonding numbers (see P-14.1). The symbol is placed before the appropriate 'a' prefix.

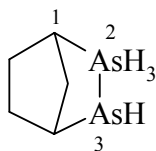
Example:



$3\lambda^4$ -thiabicyclo[3.2.1]octane (PIN)

P-23.6.2 When there is a choice for numbering, low locants are assigned to heteroatoms with nonstandard bonding numbers expressed by the λ^n symbol in order of decreasing numerical value of the bonding number; for example, in the case of phosphorus, the lower locant is given to a λ^5 phosphorus atom.

Example:

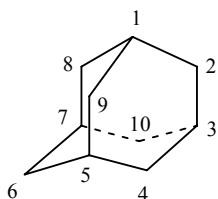


2λ⁵,3-diarsabicyclo[2.2.1]heptane (PIN)

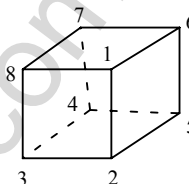
P-23.7 Retained names

The retained names adamantane and cubane are used in general nomenclature and as preferred IUPAC names. The name quinuclidine is retained for general nomenclature only (see Table 2.6).

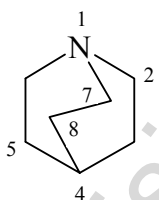
Table 2.6 Retained names for von Baeyer parent hydrides



adamantane (PIN)
tricyclo[3.3.1.1^{3,7}]decane



cubane(PIN)
pentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane



quinuclidine
1-azabicyclo[2.2.2]octane (PIN)

P-24 Spiro compounds

- P-24.0 Introduction
- P-24.1 Definitions
- P-24.2 Compounds with only monocyclic ring components
- P-24.3 Monospiro compounds containing two identical polycyclic components
- P-24.4 Three identical components spirofused together
- P-24.5 Monospiro compounds with different components at least one of which is polycyclic
- P-24.6 Unbranched polyspiro compounds with different components, one being polycyclic
- P-24.7 Branched polyspiro compounds

P-24.8 Spiro systems containing atoms with nonstandard bonding numbers

P-24.0 Introduction

This Section is based on the recent publication 'Extension and Revision of the Nomenclature for Spiro Compounds, IUPAC Recommendations 1999' (ref. 8). It supersedes Rules A-41, A-43, B-10 and B-12 in the 1979 Recommendations (ref. 1) and Rule R-2.4.3 in the 1993 Recommendations (ref. 2). The alternative methods given by Rules A-42 and B-11 in the 1979 recommendations (ref. 1) have been abandoned.

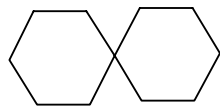
Section P-24.5.2 takes into account appropriate modifications to Section SP-4.1 of the 1999 publication (ref. 8). No other modifications have been made to the 1999 publication.

The spiro ring systems consisting only of monocyclic rings in this Section are saturated systems; for unsaturated systems, see Section P-31.1.5.1.

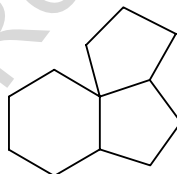
For naming substituent groups see Sections P-29 and P-32.1.2.

P-24.1 Definitions

A 'spiro union' is a linkage between two rings that consists of a single atom common to both rings. A 'free spiro union' is a linkage that constitutes the only direct union between the two rings.



a free spiro union



a non-free spiro union

The common atom is designated as the 'spiro atom'. According to the number of spiro atoms present, compounds are distinguished as monospiro, dispiro, trispiro, etc., ring systems. The following recommendations apply only to the naming of parent hydrides containing free spiro unions. For naming spiro compounds with non-free spiro unions, see nomenclature of fused systems (see P-25 and ref. 4).

Spirofusion is the creation of one, and only one, common atom between two rings or ring systems, each ring or ring system contributing one, and only one, atom. It is analogous to the *ortho*- or *ortho*- and *peri*-fusion that creates common bonds between mancude rings or ring systems. Traditionally, *ortho*- or *ortho*- and *peri*-fusion has been called 'fusion', with no reference to its specific type of fusion. To avoid any ambiguity, the term 'spiro' must always be specified when added to the term 'fusion'.

P-24.2 Spiro compounds with only monocyclic ring components

P-24.2.0 Introduction

P-24.2.1 Monospiro alicyclic hydrocarbons

P-24.2.2 Linear polyspiro alicyclic hydrocarbons

P-24.2.3 Branched polyspiro alicyclic hydrocarbons

P-24.2.4 Heterocyclic spiro compounds with only monocyclic ring components

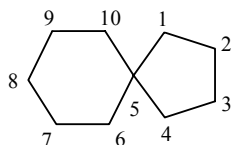
P-24.2.0 Introduction

This Section is concerned only with saturated spiro compounds that consist only of monocyclic rings. For unsaturated systems, see Section P-31.1.5.

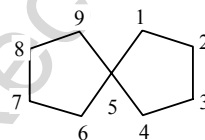
P-24.2.1 Monospiro alicyclic hydrocarbons

Monospiro parent hydrides consisting of two saturated cycloalkane rings are named by placing the nondetachable prefix 'spiro' before the name of the unbranched acyclic hydrocarbon with the same total number of skeletal atoms. The number of skeletal atoms linked to the spiro atom in each ring is indicated by arabic numbers separated by a full stop, cited in ascending order and enclosed in square brackets; this descriptor (called in these recommendations the 'von Baeyer spiro descriptor') is placed between the spiro prefix and the name of the acyclic alkane. Numbering starts in the smaller ring, if one is smaller, with a ring atom next to the spiro atom and proceeds first around that ring and then through the spiro atom and around the second ring.

Examples:



spiro[4.5]decane (PIN)

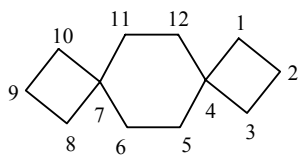


spiro[4.4]nonane (PIN)

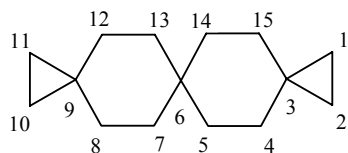
P-24.2.2 Linear polyspiro alicyclic hydrocarbons

Polyspiro parent hydrides consisting of unbranched assemblies of three or more saturated cycloalkane rings are named using the nondetachable prefixes 'dispiro', 'trispiro', etc., according to the number of spiro atoms present, cited in front of the name of the acyclic hydrocarbon that has the same number of skeletal atoms. The von Baeyer spiro descriptor indicates the number of carbon atoms linking the spiro atoms by arabic numbers that are cited in order starting at the smaller terminal ring, if one is smaller, and proceeding consecutively to the other terminal ring through each spiro atom always by the shortest path, and then back to the first spiro atom; the numbers are separated by full stops and enclosed in square brackets. The compound is numbered in the order in which the numbers of the von Baeyer spiro descriptor are cited, including spiro atoms when encountered for the first time. Each time a spiro atom is reached for the second time its locant is cited as a superscript number to the number of the preceding linking atoms.

Examples:



dispiro[3.2.3⁷.2⁴]dodecane (PIN)

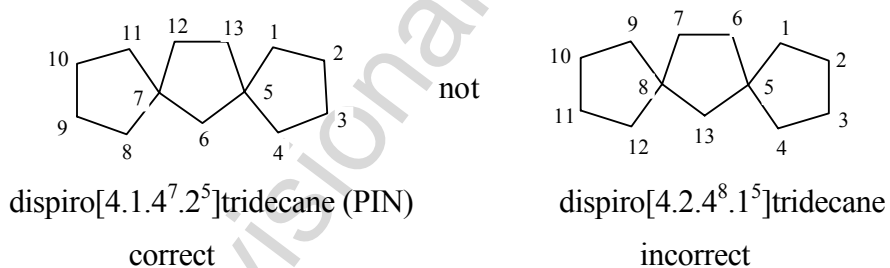


trispiro[2.2.2.2⁹.2⁶.2³]pentadecane (PIN)

The use of superscript numbers was introduced in the publication 'Extension and Revision of the Nomenclature for Spiro Compounds and IUPAC Recommendations 1999' (ref. 8). Even though they are not needed in di- or trispiro compounds their use in branched spiro systems is essential for deriving unambiguous names; therefore, it is recommended that they be used to name all polyspiro compounds, especially when IUPAC preferred names are required.

P-24.2.2.1 If there is a choice of numbers for the spiro descriptor, the smaller numbers are selected because low locants must be allocated to spiro atoms.

Examples:



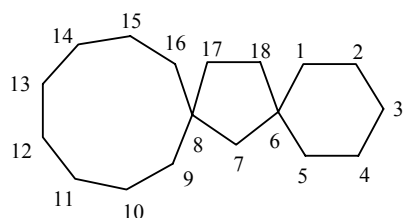
dispiro[4.1.4⁷.2⁵]tridecane (PIN)

correct

dispiro[4.2.4⁸.1⁵]tridecane

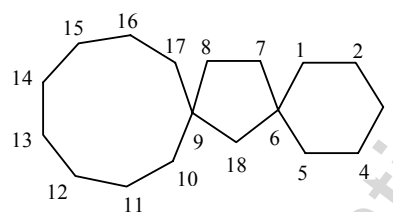
incorrect

(in the correct name, the number set '4,1' is lower than '4,2' and/or the spiro atom locant set 5,7 is smaller than 5,8)



dispiro[5.1.8⁸.2⁶]octadecane (PIN)

correct



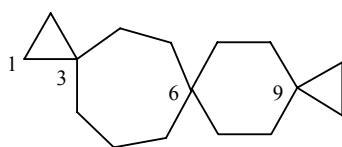
dispiro[5.2.8⁹.1⁶]octadecane

incorrect

(in the correct name, the number set '5,1' is lower than '5,2' and/or the spiro atom locant set 6,8 is smaller than 6,9)

P-24.2.2.2 If there is still a choice of numbering, the numbers of the von Baeyer descriptors are considered in their order of citation. The name is selected with lower numbers at the first point of difference.

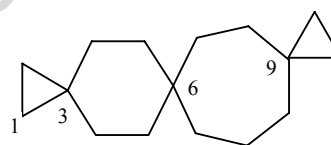
Example:



trispiro[2.2.2.2⁹.2⁶.3³]hexadecane (PIN)

correct

not



trispiro[2.2.2.2⁹.3⁶.2³]hexadecane

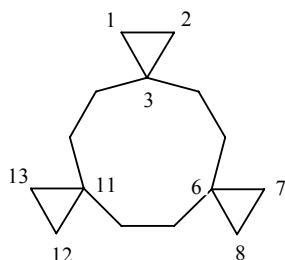
incorrect

(in the correct name, the number set '2,2,2,2⁹,2⁶,3³' is lower than '2,2,2,2⁹,3⁶,2³')

P-24.2.3 Branched polyspiro alicyclic hydrocarbons

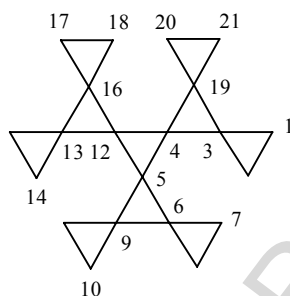
Branched polyspiro hydrocarbons composed only of cycloalkane rings are named using 'dispiro', 'trispiro', etc. before the name of the acyclic hydrocarbon corresponding to the total number of carbon atoms present. The von Baeyer spiro descriptor indicates the number of carbon atoms linking the spiro atoms by lower case arabic numbers that are cited in order starting at the smallest terminal ring, if one is smallest, proceeding consecutively to succeeding terminal rings through each spiro atom always by the shortest path, and then back to the first spiro atom; the numbers are separated by full stops and enclosed in square brackets. The compound is numbered in the order in which the numbers of the spiro von Baeyer descriptor are cited, including spiro atoms when encountered for the first time. Each time a spiro atom is reached for the second time its locant is cited as a superscript number to the preceding number of linking atoms.

Examples:



trispiro[2.2.2⁶.2.2¹¹.2³]pentadecane (PIN)

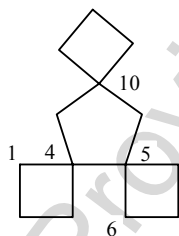
(the importance of superscripts is illustrated by this example and the second example in P-24.2.2; without the superscripts these different compounds would have identical names)



nonaspiro[2.0.0.0.2⁶.0.2⁹.0⁵.0.0.2¹³.0.2¹⁶.0¹².0⁴.0.2¹⁹.0³]henicosane (PIN)

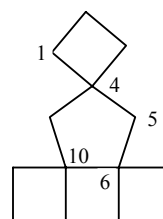
P-24.2.3.1 If there is a choice for numbering, lowest locants are assigned to the spiro atoms.

Example:



trispiro[3.0.3⁵.1.3¹⁰.1⁴]tetradecane (PIN)

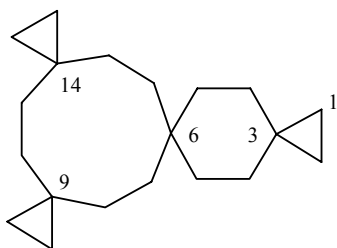
correct



trispiro[3.1.3⁶.0.3¹⁰.1⁴]tetradecane

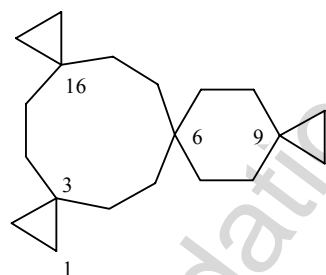
incorrect

(in the correct name, the number set of the descriptor '3,0' is lower than '3,1' and/or the spiro atom locant set '4,5,10' is lower than '4,6,10')



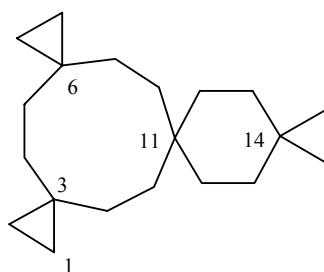
tetraspiro[2.2.2.2⁹.2.2¹⁴.2⁶.2³]icosane (PIN)

correct



tetraspiro[2.2.2.2⁹.2.2¹⁶.2⁶.2³]icosane

incorrect



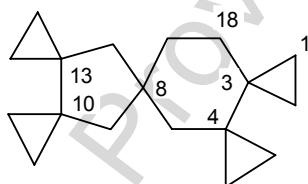
tetraspiro[2.2.2.2⁶.2.2.2¹⁴.2¹¹.2³]icosane (PIN)

incorrect

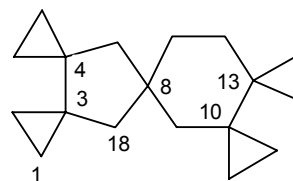
(in the correct name, the spiro locant set '3,6,9,14' is lower than '3,6,9,16' or '3,6,11,14')

P-24.2.3.2 If there is still a choice of numbering, the numbers of the von Baeyer descriptor are considered in their order of citation. The correct name has the lower numbers at first point of difference.

Example:



not



pentaspiro[2.0.2⁴.1.1.2¹⁰.0.2¹³.1⁸.2³]octadecane (PIN) pentaspiro[2.0.2⁴.1.1.2¹⁰.0.2¹³.2⁸.1³]octadecane

correct

incorrect

(in the correct name, the number set of the descriptor '2,0,2,1,1,2,0,2,1,2' is lower than the number set '2,0,2,1,1,2,0,2,2,1', the number '1' being lower than '2' at the ninth position)

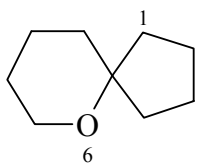
P-24.2.4 Heterocyclic spiro compounds

- P-24.2.4.1 Heterocyclic spiro compounds named by skeletal replacement ('a') nomenclature
- P-24.2.4.2 Homogeneous heterocyclic spiro compounds with only monocyclic components
- P-24.2.4.3 Heterocyclic spiro compounds with only monocyclic components composed of alternating heteroatoms

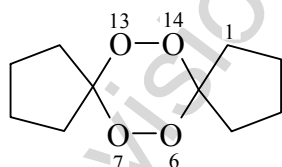
P-24.2.4.1 Heterocyclic spiro compounds named by skeletal replacement ('a') nomenclature

P-24.2.4.1.1 When heteroatoms are present in a spiro system composed of only monocyclic rings, skeletal replacement ('a') nomenclature is used to name the heterocyclic system. The name of the corresponding hydrocarbon is first constructed as described above (P-24.2). Heteroatoms are then introduced by using the general principles of skeletal replacement ('a') nomenclature. The numbering of the spiro hydrocarbon is never modified by the introduction of heteroatoms, but low locants must be attributed to heteroatoms if there is a choice.

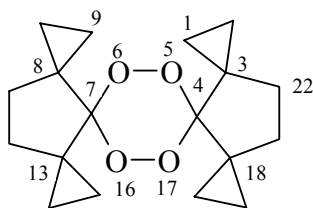
Examples:



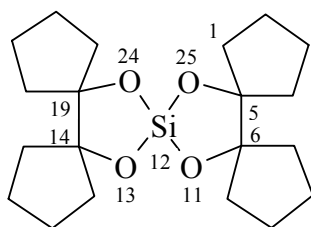
6-oxaspiro[4.5]decane (PIN)
(not 10-oxaspiro[4.5]decane)



6,7,13,14-tetraoxadispiro[4.2.4⁸.2⁵]tetradecane (PIN)



5,6,16,17-tetraoxahexaspiro[2.0.2.0.2⁸.2.2¹³.0⁷.2⁴.0.2¹⁸.2³]docosane (PIN)

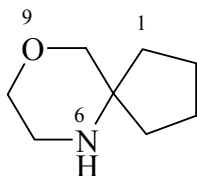


11,13,24,25-tetraoxa-12-silapentaspiro[4.0.4⁶.1.1.4¹⁴.0.4¹⁹.1¹².1⁵]pentacosane (PIN)

P-24.2.4.1.2 If there is a choice of name or numbering due to heteroatoms, the following criteria are considered in order until a decision is reached.

- (a) Low locants are allocated to heteroatoms as a set regardless of the kind of heteroatom.

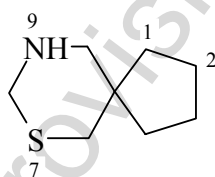
Example:



9-oxa-6-azaspiro[4.5]decane (PIN)

- (b) If there is still a choice, low locants are assigned in accord with the following decreasing seniority order of heteroatoms: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Example:

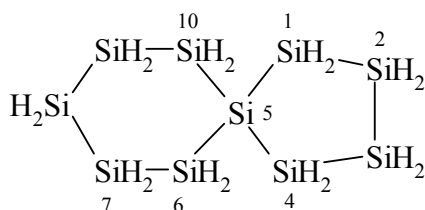


7-thia-9-azaspiro[4.5]decane (PIN)

P-24.2.4.2 Homogeneous heterocyclic spiro compounds with only monocyclic components

Heterocyclic spiro compounds with only monocyclic components and composed entirely of the same heteroatom are named as described in P-24.2 using the name of the homogeneous heteroacyclic parent hydride that has the same total number of skeletal heteroatoms. This method is preferred to skeletal replacement ('a') nomenclature described in P-24.2.4.1, in which the total number of heteroatoms is indicated by a numerical term. In either method it is not necessary to give the location of the heteroatoms because all positions are modified by the same heteroatom. The former method produces preselected parent hydride names.

Example:



spiro[4.5]decasilane (preselected name; see P-12.2)
decasilaspiro[4.5]decane

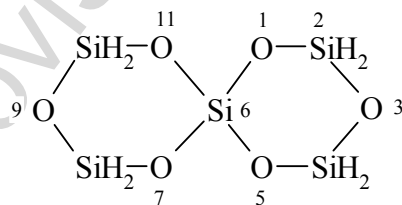
P-24.2.4.3 Heterocyclic spiro compounds consisting only of monocyclic rings and having alternating skeletal heteroatoms are named by two methods.

- (a) By citing a prefix such as 'spiro', 'dispiro', etc., before a von Baeyer descriptor (indicating the numbers of heteroatoms linked to each spiro atom in each ring cited in increasing order and separated by a full stop) enclosed in square brackets followed successively by:
- a multiplying prefix ('di', 'tri', etc) denoting the number of heteroatoms of the first cited 'a' term that follows;
 - the 'a' terms of the hetero atoms, cited in the reverse seniority order for 'a' prefixes (see P-21.2.3.1), for example, Si before O);
 - the ending 'ane'. The hetero spiro system is numbered as is the corresponding hydrocarbon.

(b) By skeletal replacement ('a') nomenclature as described in P-24.2.4.1.

Method (b) generates preselected names.

Example:



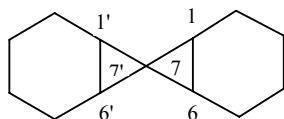
spiro[5.5]pentasiloxane
1,3,5,7,9,11-hexaoxa-2,4,6,8,10-pentasilaspiro[5.5]undecane
(preselected name; see P-12.2)

P-24.3 Monospiro compounds containing two identical polycyclic components

P-24.3.1 Monospiro compounds consisting of two identical polycyclic components are named by placing the nondetachable prefix 'spirobi' before the name of the component ring system enclosed in square brackets. The established numbering system of the polycyclic component system is retained

with one system having primed locants. The location of the spiro atom is indicated in the name by the appropriate locants (unprimed first) placed at the front of the name.

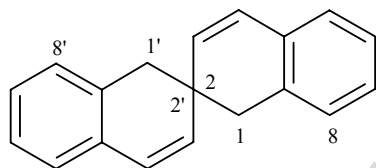
Example:



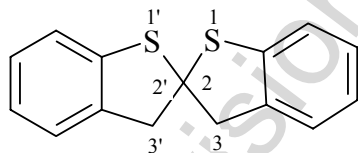
7,7'-spirobi[bicyclo[4.1.0]heptane] (PIN)

P-24.3.2 Where appropriate the maximum number of noncumulative double bonds is added (i.e., the system is made mancude) after construction of the whole skeleton. No indicated hydrogen is cited when none is present in the spiro system. If indicated hydrogen is needed, it is cited in front of the spiro atom locants.

Examples:

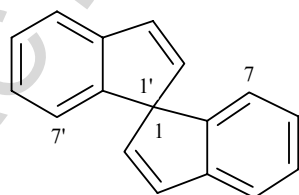


1H,1'H-2,2'-spirobi[naphthalene] (PIN)

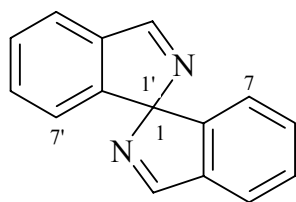


3H,3'H-2,2'-spirobi[[1]benzothiophene] (PIN)

Note: The double set of brackets in this name occurs because the spiro name requires them and brackets are used to enclose locants belonging to component names (see P-16.4.2.2).



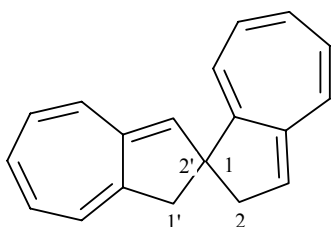
1,1'-spirobi[indene] (PIN)



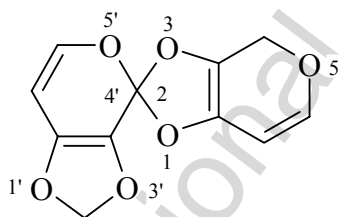
1,1'-spirobi[isoindole] (PIN)

P-24.3.3 If there is a choice for assigning primed locants, the lower number at the spiro atom is unprimed.

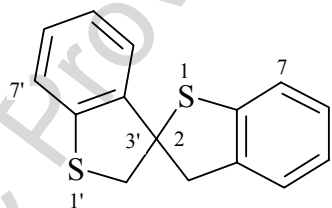
Examples:



1'*H*,2*H*-1,2'-spirobi[azulene] (PIN)

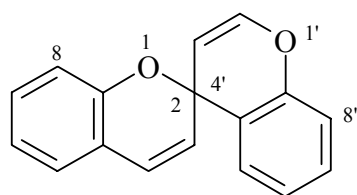


4*H*-2,4'-spirobi[[1,3]dioxolo[4,5-*c*]pyran] (PIN)



2'*H*,3*H*-2,3'-spirobi[[1]benzothiophene] (PIN)

(the indicated hydrogen at position 2' may be omitted in general nomenclature, but it must be cited in the preferred IUPAC name)

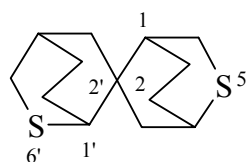


2,4'-spirobi[chromene] (PIN)

P-24.3.4 Heterocyclic 'spirobi' compounds named by skeletal replacement ('a') nomenclature

When components of 'spirobi' compounds are named by von Baeyer nomenclature, heteroatoms are indicated by skeletal replacement ('a') nomenclature. The spirobi- system is named as the saturated bi- or polycyclic alicyclic hydrocarbon and the heteroatoms are denoted by 'a' prefixes cited at the front of the completed 'spirobi' hydrocarbon name. If there is a choice, low locants are given to the spiro atom, then to the heteroatoms as described in Section P-24.2.4.1.

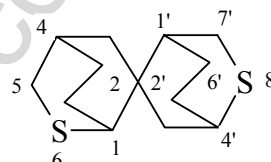
Examples:



(I)

correct

not

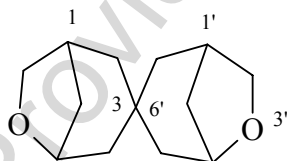


(II)

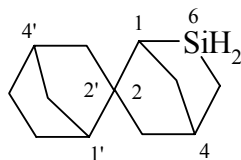
incorrect

5,6'-dithia-2,2'-spirobi[bicyclo[2.2.2]octane] **(I)** (PIN)

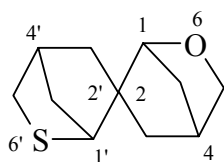
[not 6,8'-dithia-2,2'-spirobi[bicyclo[2.2.2]octane] **(II)**; the set of locants '5,6' in **(I)** is lower than '6,8' in **(II)**]



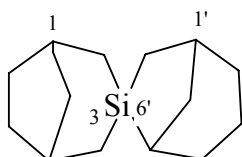
3',6-dioxa-3,6'-spirobi[bicyclo[3.2.1]octane] (PIN)



6-sila-2,2'-spirobi[bicyclo[2.2.1]heptane] (PIN)



6-oxa-6'-thia-2,2'-spirobi[bicyclo[2.2.1]heptane] (PIN)

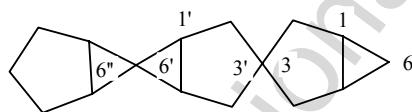


3-sila-3,6'-spirobi[bicyclo[3.2.1]octane] (PIN)

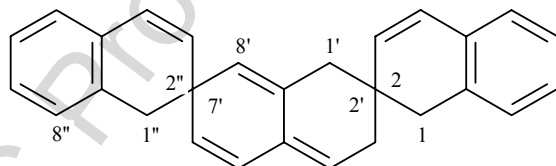
P-24.4 Three identical polycyclic components spirofused together

P-24.4.1 Dispiro compounds with three identical polycyclic components are named by placing the nondetachable prefix 'dispiroter' before the name of the component ring system enclosed in square brackets. The Latin multiplicative prefix 'ter' (see P-14.2.4) is used to indicate the repetition of identical components. Locants for the middle component are primed and for the third component double primed. The spiro atoms are indicated in front of the name by two pairs of locants separated by a colon. Indicated hydrogen is cited in front of these locants, if needed.

Examples:



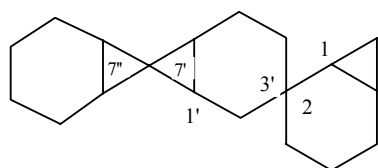
3,3':6',6''-dispiroter[bicyclo[3.1.0]hexane] (PIN)



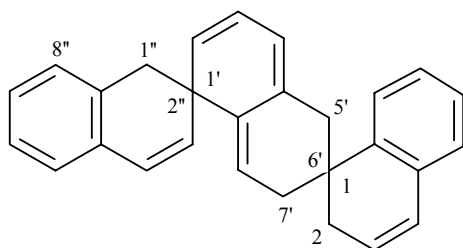
1H,1'H,1''H,3'H-2,2':7',2''-dispiroter[naphthalene] (PIN)

P-24.4.2 If there is a choice for locants, the lowest set of locants for all spiro atoms is selected when compared as a set in increasing order and, if there is a further choice, in order of citation in the name.

Examples:



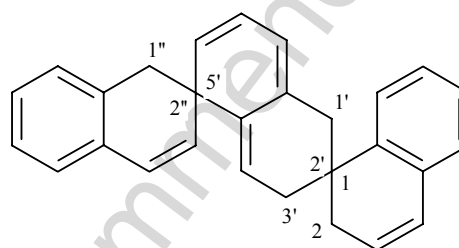
2,3':7',7''-dispiroter[bicyclo[4.1.0]heptane] (PIN)



(I)

correct

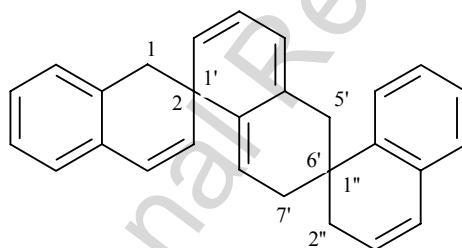
not



(II)

incorrect

nor



(III)

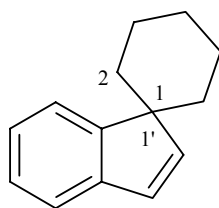
incorrect

1''H,2H,5'H,7'H-1,6':1',2''-dispiroter[naphthalene] (I) (PIN)
 [not 1''H,1''H,2H,3'H-1,2':5',2''-dispiroter[naphthalene] (II),
 nor 1H,2''H,5''H,7''H-2,1':6',1''-dispiroter[naphthalene] (III);
 the locant set '1,1',2',6'' in (I) is lower than '1,2',2'',5'' in
 (II) or '1',1'',2,6'' in (III)]

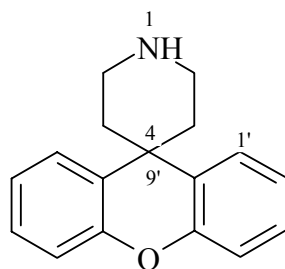
P-24.4.3 Three identical heterocyclic components spiro fused together

Dispiro compounds with three identical heterocyclic components may be named:

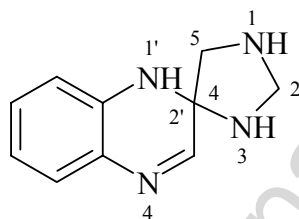
- by using heterocyclic monocyclic or polycyclic parent components in the same way as for 'spiroter' hydrocarbons (see P-24.4.1). The numbering depends on the fixed numbering of the heterocyclic components;
- by skeletal replacement ('a') nomenclature when the components are polycyclic von Baeyer compounds; the numbering of the 'spiroter' von Baeyer hydrocarbon remains unchanged.



spiro[cyclohexane-1,1'-indene] (PIN)



spiro[piperidine-4,9'-xanthene] (PIN)

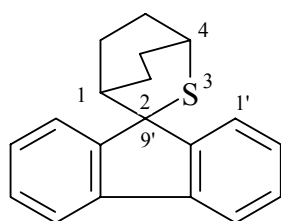


1'*H*-spiro[imidazoline-4,2'-quinoxaline] (PIN)

P-24.5.2 Monospiro compounds with different components at least one being polycyclic and at least one requiring the use of skeletal replacement ('a') nomenclature are named as in P-24.5.1; then, the 'a' prefixes are introduced and cited before the 'spiro' term.

This is a change from the publication given in ref. 8 (see SP-4.1) in which the 'a' prefixes were kept with the component ring system.

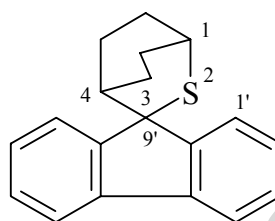
Examples:



(I)

correct

not

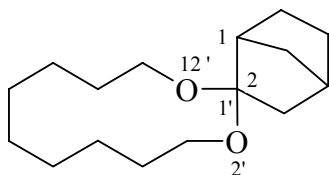


(II)

incorrect

3-thiaspiro[bicyclo[2.2.2]octane-2,9'-fluorene] **(I)** (PIN)
 [not 2-thiaspiro[bicyclo[2.2.2]octane-3,9'- fluorene] **(II)**;
 the locant set '2,9' in **(I)** is lower than '3,9' in **(II)**]

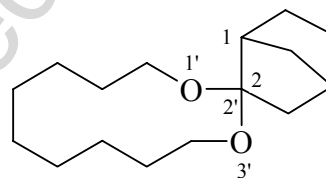
(the format of the 'correct' name as given in SP-4.1 in ref. 8,
 spiro[fluorene-9,2'-[3]thiabicyclo[2.2.2]octane], is no longer
 recommended)



(I)

correct

not



(II)

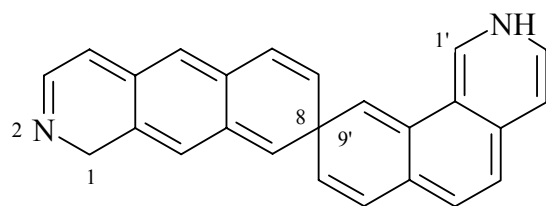
incorrect

2',12'-dioxaspiro[bicyclo[2.2.1]heptane-2,1'-(cyclododecane)] **(I)** (PIN)
 [not 1',3'-dioxaspiro[bicyclo[2.2.1]heptane-2,2'-(cyclododecane)] **(II)**;
 the spiro atom of the monocyclic hydrocarbon component is given preference
 for low locant]

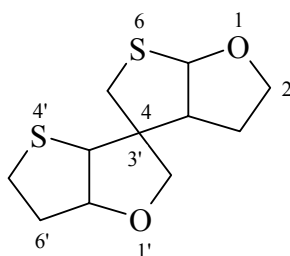
(the format of the 'correct' name as given in SP-4.1, ref. 8),
 spiro[bicyclo[2.2.1]heptane-2,1'-[2,12]dioxacyclododecane]
 is no longer recommended]

P-24.5.3 Alphanumerical order, as described in Section P-14.5, is used when necessary. When Roman letters are inadequate to distinguish alphabetically between two components, criteria based on lower italic fusion letters and numbers, heteroatom locants, and von Baeyer descriptor numbers are used, as appropriate. Locants present in bicyclic fused benzo compounds are directly cited at the front of the spiro name when they correspond to the numbering of the spiro compound; when they do not correspond to those of the spiro compound, they are placed in brackets (see third and fourth examples below).

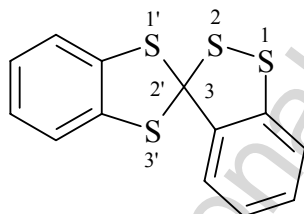
Examples:



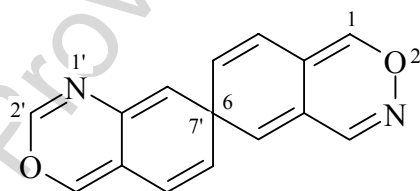
1*H*,2'*H*-spiro[benzo[*g*]isoquinoline-8,9'-benzo[*h*]isoquinoline] (PIN)
(benzo[*g*]... before benzo[*h*]...)



2'*H*,5*H*-spiro[thieno[2,3-*b*]furan-4,3'-thieno[3,2-*b*]furan] (PIN)
(...[2,3-*b*]... before ...[3,2-*b*]...)



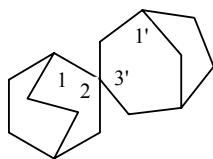
spiro[[1,2]-benzodithiole-3,2'-[1,3]benzodithiole] (PIN)
(1,2-benzo... before 1,3-benzo...)



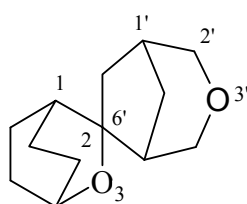
spiro[[2,3]-benzoxazine-6,7'-[3,1]benzoxazine] (PIN)
(2,3-benzoxazine before 3,1-benzoxazine)

P-24.5.4 In the case of components modified by skeletal replacement ('a') nomenclature, Rules P-24.5.2 and P-24.5.3 are applied to name the compound before skeletal replacement ('a') nomenclature is applied as described in P-24.5.2. The names of components modified by skeletal replacement ('a') nomenclature must not be used; thus Rule P-24.5.3 must be applied when required.

Examples:



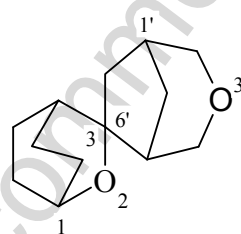
spiro[bicyclo[2.2.2]octane-2',3-bicyclo[3.2.1]octane] (PIN)
[bicyclo[2.2.2]octane before bicyclo[3.2.1]octane; the descriptor set '2.2.2' is lower than '3.2.1' (see P-14.5.4)]



(I)

correct

not



(II)

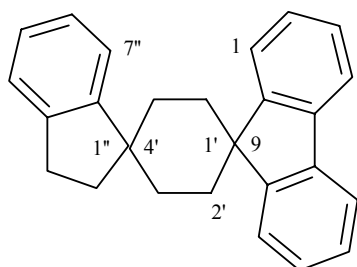
incorrect

3,3'-dioxaspiro[bicyclo[2.2.2]octane-2,6'-bicyclo[3.2.1]octane] **(I)** (PIN)
[not 2,3'-dioxaspiro[bicyclo[2.2.2]octane-3,6'-bicyclo[3.2.1]octane] **(II)**;
spiro fusion is preferred to 'a' prefixes for low locants and the locant set '2,6' in **(I)** is lower than '3,6' in **(II)**]

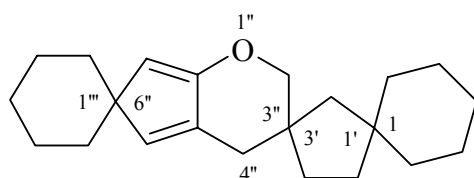
P-24.6 Unbranched polyspiro compounds with different components, one being polycyclic

Unbranched polyspiro compounds with at least two different components and at least one of which is polycyclic are named by placing the component names in order of their occurrence in the structure beginning with the terminal component lower in alphabetical order and enclosing with square brackets. A nondetachable prefix indicating the number of spiro atoms ('dispiro', 'trispiro', etc.) is placed in front of the enclosed component names. Locants of the first cited component are unprimed, the next one is primed, and so on; accordingly, locants required by the names of the second and later components are enclosed in square brackets. The positions of the spiro atoms are indicated by the appropriate pair of locants separated by a comma and placed between each pair of component ring system names. Indicated hydrogen is used as needed and cited in front of the 'dispiro', 'trispiro', etc., prefix. If both terminal ring systems are the same, the order for citation of components is determined by comparing the pair of second components from the end of the structure, and so on (See section SP-5 in ref. 8 for further discussion).

Examples:



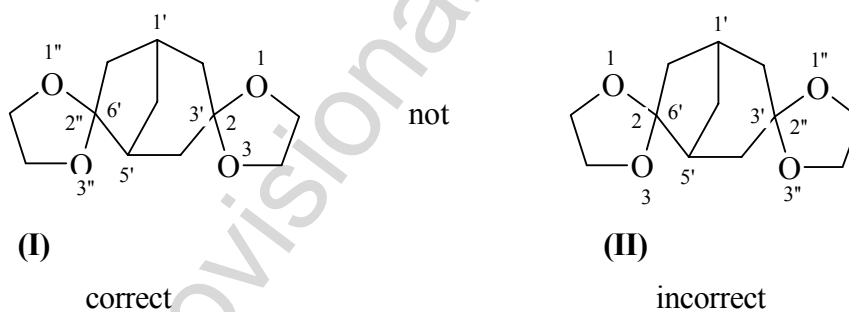
dispiro[fluorene-9,1'-cyclohexane-4',1''-indene] (PIN)



2''H,4''H-trispiro[cyclohexane-1,1'-cyclopentane-3',3''-cyclopenta[*b*]pyran-6'',1'''-cyclohexane] (PIN)

P-24.6.1 If there is a choice of locants, the lowest set of locants for all spiro atoms is selected when compared in increasing order and, if there is still a choice, in order of their citation in the name (see P-24.2.4.1).

Example:



dispiro[1,3-dioxolane-2,3'-bicyclo[3.2.1]octane-6',2''-[1,3]dioxolane] **(I)** (PIN)
 [not dispiro[1,3-dioxolane-2,6'-bicyclo[3.2.1]octane-3'-2''-[1,3]dioxolane]**(II)**;
 the locant sets '2,2'',3',6'' are identical, but in the name the order of citation
 '2,3',6',2'' in **(I)** is lower than '2,6',3',2'' in **(II)**]

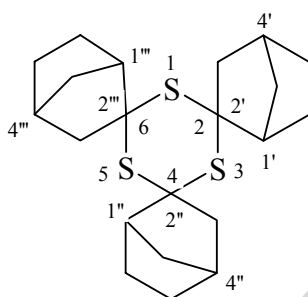
Note: The 'correct' name above is constructed in accordance with the traditional method, and is preferred. An alternative name, dispiro[bicyclo[3.2.1]octane-2,3':6',2''-bis([1,3]dioxolane), could be considered as an adaptation of multiplicative nomenclature (see also P-24.7).

P-24.7 Branched polyspiro compounds

When three or more components are spirofused to another single component, the system is described as a branched spirofused system. Terminal components have only one spiro atom.

P-24.7.1 When a central component is spirofused to three or more identical terminal components, the central component is cited first and its locants are unprimed. The terminal components are cited with the appropriate multiplicative prefix ('tris', 'tetrakis', etc.) and locants primed, double primed, etc. in accordance with the lowest possible locants of the spiro atoms of the central component. The spiro atoms are indicated by pairs of locants separated by a colon. Indicated hydrogen is cited as necessary in front of the appropriate spiro prefix.

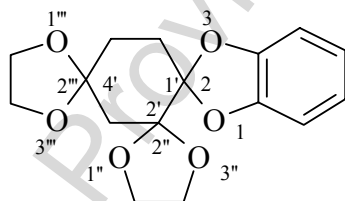
Example:



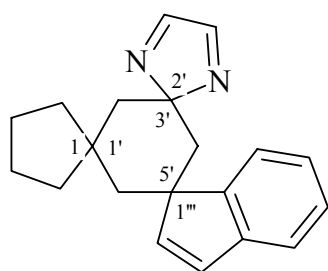
trispiro[1,3,5-trithiane-2,2':4,2'':6,2'''-tris(bicyclo[2.2.1]heptane)] (PIN)

P-24.7.2 When two or more different terminal components are spirofused to a central component, the alphabetically earliest is cited first with a multiplicative prefix, if appropriate, followed by the central component and then the remaining terminal component(s) in alphabetical order, the first cited being spirofused to the lowest numbered spiro position of the central component.

Examples:



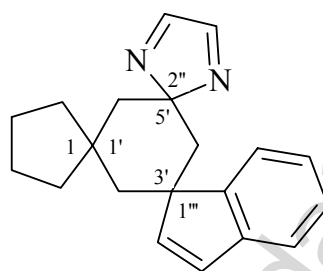
trispiro[1,3-benzodioxole-2,1'-cyclohexane-2',2'':4',2'''-bis([1,3]dioxolane)] (PIN)



(I)

correct

not



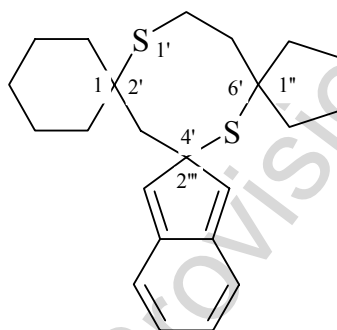
(II)

incorrect

trispiro[cyclopentane-1,1'-cyclohexane-3'-2''-imidazole-5',1'''-indene] **(I)** (PIN)
 [not trispiro[cyclopentane-1,1'-cyclohexane-5',2''-imidazole-3',1'''-indene] **(II)**;
 the locant sets '1,1',1''',2'',3',5'' in both **(I)** and **(II)** are the same, but in the name
 the order of citation, '1,1',3',2'',5',1'''' in **(I)** is lower than '1,1',5',2'',3',1''''
 in **(II)** (see P-24.7.3)]

P-24.7.3 If there is a choice of locants, the lowest set of locants for all spiro atoms is selected when compared as a set in increasing order, and, if still undecided, in their order of citation in the name. If a choice still remains, criteria about heteroatoms and indicated hydrogen are taken into consideration (see Section SP-3.2 in ref 8).

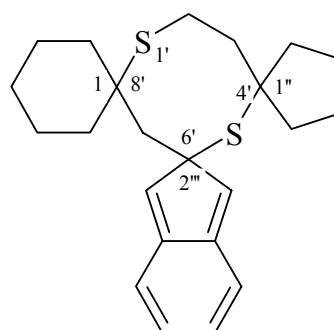
Example:



(I)

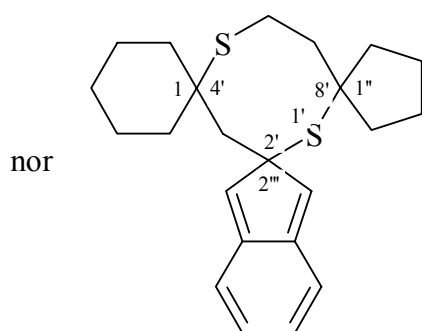
correct

not



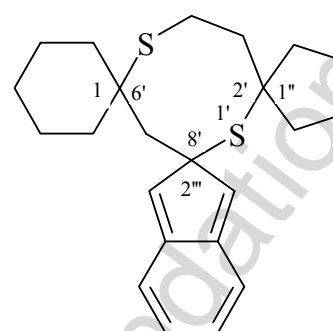
(II)

incorrect



(III)

incorrect



(IV)

incorrect

trispiro[cyclohexane-1,2'-[1,5]dithiocane-6',1''-cyclopentane-4',2'''-indene] (I) (PIN)
[not trispiro[cyclohexane-1,8'-[1,5]dithiocane-4',1''-cyclopentane-6',2'''-indene] (II);
nor trispiro[cyclohexane-1,4'-[1,5]dithiocane-8',1''-cyclopentane-2',2'''-indene] (III);
nor trispiro[cyclohexane-1,6'-[1,5]dithiocane-2',1''-cyclopentane-8',2'''-indene] (IV);
the locant set '1,1'',2',2''',4',6'' ' in (I) is lower than '1,1'',2''',4',6',8'' ' in (II).
'1,1'',2',2''',4',8'' ' in (III), or '1,1'',2',2''',6',8'' ' in (IV)]

P-24.8 Spiro systems containing atoms with nonstandard bonding numbers

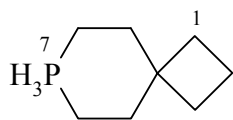
The λ -convention, characterized by the symbol λ^n , is used to identify heteroatoms with nonstandard bonding numbers (see P-14.1). The symbol is placed at the front of the complete name or before the 'a' prefix for the atom to which it refers.

- P-24.8.1 Spiro compounds with only monocyclic ring components
- P-24.8.2 Monospiro compounds containing two identical polycyclic components
- P-24.8.3 Three identical components with one nonstandard spiro atom
- P-24.8.4 Monospiro compounds with different components at least one of which is polycyclic and a nonstandard spiro atom
- P-24.8.5 Unbranched polyspiro compounds with different components at least one of which is polycyclic and at least one nonstandard spiro atom
- P-24.8.6 Branched spiro compounds with at least one polycyclic component

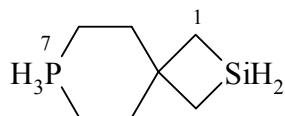
P-24.8.1 Spiro compounds with only monocyclic ring components

P-24.8.1.1 Heteroatoms having nonstandard bonding numbers receive locants in accordance with the numbering of the corresponding spiro hydrocarbon.

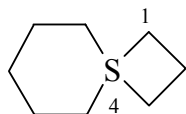
Examples:



7λ⁵-phospha-spiro[3.5]nonane (PIN)



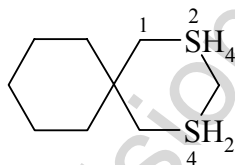
7λ⁵-phospha-2-silasp[3.5]nonane (PIN)



4λ⁴-thiaspiro[5.3]nonane (PIN)

P-24.8.1.2 If there is a choice, lower locants are assigned to heteroatoms with the higher bonding numbers, for example, the lower number is assigned to a λ⁶ heteroatom rather than to a λ⁴ heteroatom.

Example:

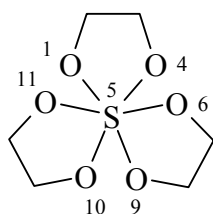


2λ⁶-thia-4λ⁴-thiaspiro[5.5]undecane (PIN)

P-24.8.1.3 Spiro ring systems composed only of three monocyclic rings and a nonstandard spiro atom.

P-24.8.1.3.1 Ring systems consisting of three monocyclic rings and one nonstandard spiro atom (e.g., a λ⁶ spiro atom) are named by placing the prefix 'spiro' before the name corresponding to an acyclic hydrocarbon with the same total number of atoms in the spiro ring system. Heteroatoms are indicated by 'a' prefixes and the nonstandard bonding number by the lambda symbol (see P-14.1). In the von Baeyer spiro descriptor, the locant of the spiro atom is used as a superscript number to indicate each time the spiro atom is revisited.

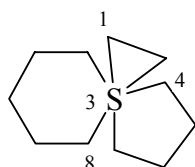
Example:



1,4,6,9,10,13-hexaoxa-5 λ^6 -thiaspiro[4.4⁵.4⁵]tridecane (PIN)

P-24.8.1.3.2 If there is a choice for numbering, a small ring is numbered before a larger ring.

Example:

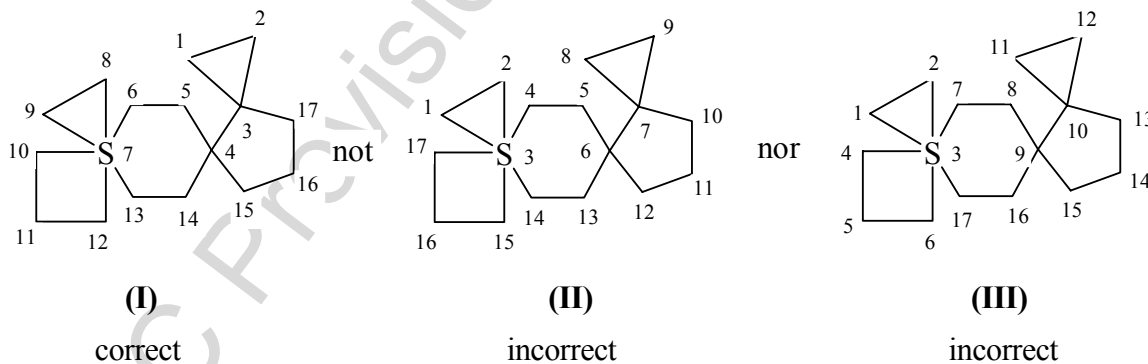


3 λ^6 -thiaspiro[2.4³.5³]dodecane (PIN)

P-24.8.1.4 Polyspiro systems which include three monoalicyclic rings with one nonstandard hetero spiro atom as well as other spiro fusions are named using a combination of methods for naming the polyspiro hydrocarbons and for indicating heteroatoms with nonstandard bonding numbers. If there is a choice for numbering, the following criteria are considered in order until a decision is made.

(a) Low numbers are selected for spiro atoms.

Example:



7 λ^6 -thiatrispiro[2.0.2.2⁷.3⁷.2⁴.3³]heptadecane **(I)** (PIN)

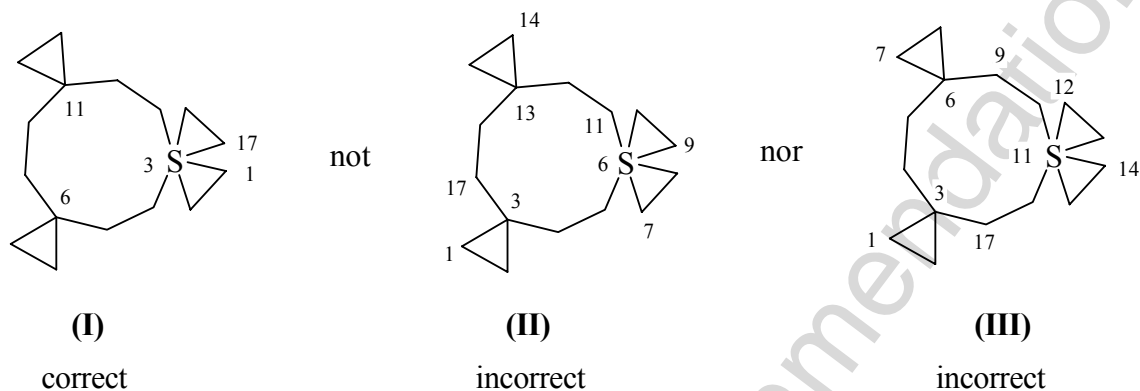
[not 3 λ^6 -thiatrispiro[2.4³.2.0.2¹⁰.3⁹.2³.3³]heptadecane **(II)**;

nor 3 λ^6 -thiatrispiro[2.4³.2.0.2¹⁰.3⁹.2³.3³]heptadecane **(III)**;

the locant set for the spiro atoms in **(I)**, '3,4,7', is lower than '3,6,7' in **(II)** or '3,9,10' in **(III)**]

(b) Low numbers are selected for spiro atoms connecting three rings.

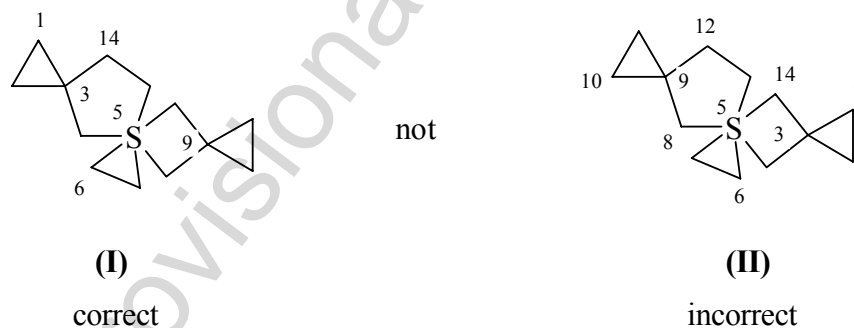
Example:



$3\lambda^6$ -thiatripiro[2.2.2⁶.2.2¹¹.2³.2³]heptadecane **(I)** (PIN)
 [not $6\lambda^6$ -thiatripiro[2.2.2⁶.2⁶.2.2¹³.2³]heptadecane **(II)**;
 nor $11\lambda^6$ -thiatripiro[2.2.2⁶.2.2¹¹.2¹¹.2³]heptadecane **(III)**;
 the locant '3' for the spiro atom connecting three rings in **(I)**
 is lower than '6' in **(II)** or '11' in **(III)**]

(c) Low numbers are selected for the von Baeyer spiro descriptor in order of citation.

Example:

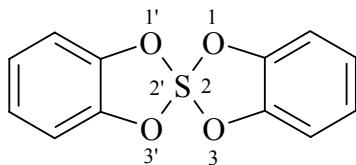


$5\lambda^6$ -thiatripiro[2.1.2⁵.1.2⁹.1⁵.2³]tetradecane **(I)** (PIN)
 [not $5\lambda^6$ -thiatripiro[2.1.2⁵.1.2⁹.2⁵.1³]tetradecane **(II)**;
 the spirodescriptor set '2,1,2,1,2,1,2' in **(I)**, is lower
 than '2,1,2,1,2,2,1' in **(II)**]

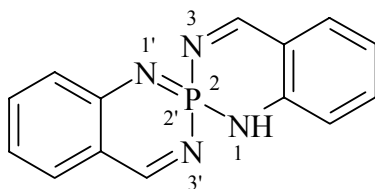
P-24.8.2 Monospiro compounds containing two identical polycyclic systems

The λ^n symbol is placed at the front of the complete name formed from the names of two identical components including the heteroatoms in their name. If indicated hydrogen atoms are required, they are placed before the λ symbol. When there is a choice, the locant of the first cited component is used for indicated hydrogen.

Examples:



$2\lambda^4$ -2,2'-spirobi[[1,3,2]benzodioxathiole] (PIN)

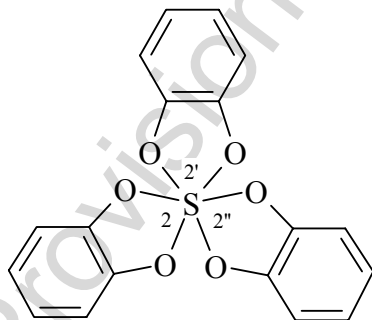


1H-2 λ^5 -2,2'-spirobi[1,3,2-benzodiazaphosphinine] (PIN)

P-24.8.3 Three identical polycyclic components with one nonstandard spiro atom

Ring systems composed of three identical polycyclic components and only one spiro atom are named by placing the prefix spiroter- before the name of the polycyclic component enclosed in square brackets. The three spiro locants are cited at the front of the name preceded by the λ -symbol with its locant.

Example:



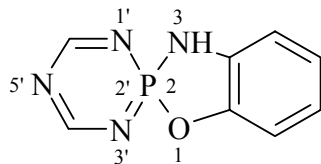
$2\lambda^6$ -2,2',2''-spiroter[[1,3,2]benzodioxathiole] (PIN)

P-24.8.4 Monospiro compounds containing a nonstandard spiro atom and different components at least one of which is polycyclic.

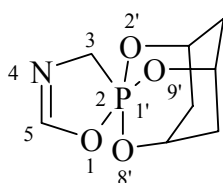
P-24.8.4.1 Monospiro ring systems composed of two different ring systems and a spiro heteroatom with a nonstandard bonding number are named by placing the prefix spiro in front of the names of the components in alphabetical order and with appropriate spiro locants. The lowest locant (unprimed) is used to denote the spiro-fusion and the appropriate λ symbol is placed at the front of the name. Indicated hydrogen, if necessary, is added in front of the λ symbol. Any additional atom with a

nonstandard bonding number is treated as a part of the name of the heterocycle; the λ symbol is cited with the appropriate locant.

Examples:

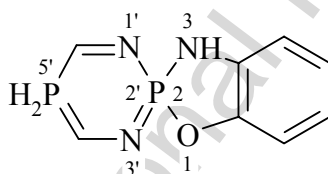


3*H*-2 λ^5 -spiro[1,3,2-benzoxazaphosphole-2,2'-[1,3,5,2]triazaphosphinine] (PIN)



3*H*- λ^5 -spiro[1,4,2-oxazaphosphole-2,1'-[2,8,9]trioxa[1]phosphaadamantane] (PIN)

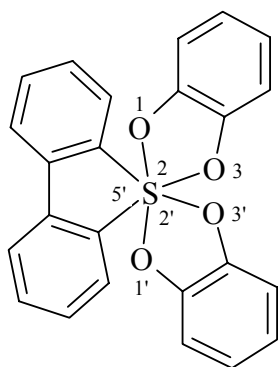
3*H*- λ^5 -spiro[1,4,2-oxazaphosphole-2,1'-[2,8,9]trioxa[1]phosphatrimethyldecane] (adamantane, a retained name, is preferred to its systematic von Baeyer name)



3*H*-2 λ^5 -spiro[1,3,2-benzoxazaphosphole-2,2'-[1,3,2,5 λ^5]diazadiphosphinine] (PIN)

P-24.8.4.2 When three components, represented by two different individual compounds, are present, the name of the component that is cited second is placed in parentheses to highlight this unusual situation.

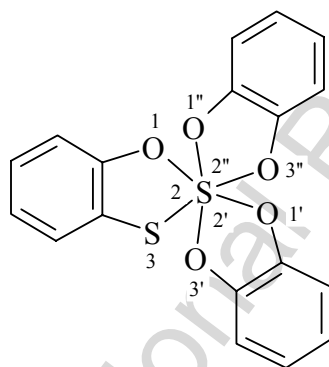
Example:



$2\lambda^6$ -spiro[1,3,2-benzodioxathiole-2,2'-(1,2,3)benzoxadithiole]-2,5''-dibenzo[*b,d*]thiophene] (PIN)

P-24.8.4.3 Two identical components are denoted by the prefix 'bis'.

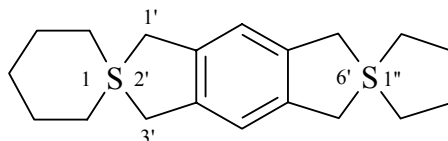
Example:



$2\lambda^6$ -spiro[bis([1.3.2]benzodioxathiazole)-2,2':2,2''-[1,2,3]benzoxadithiole] (PIN)

P-24.8.5 Unbranched polyspiro compounds with different components at least one of which is polycyclic and with at least one nonstandard spiro atom are named using the method described in P-24.6. The λ -symbol denoting a spiro junction is associated with the least primed locants and placed in front of the name; it is preceded by indicated hydrogen(s), as needed.

Example:

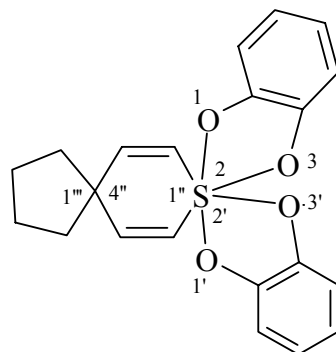


$1'H,3'H-1\lambda^4,6'\lambda^4$ -dispiro[thiane-1,2'-benzo[1,2-*c*:4,5-*c'*]dithiophene-6',1''-thiolane] (PIN)

P-24.8.6 Branched spiro compounds with at least one polycyclic component

If two or more different terminal components are spirofused to a central component, the alphabetically earliest is cited first with multiplicative prefixes, if appropriate, followed by the central component and the remaining terminal components in alphabetical order. The λ symbol is placed at the front of the complete name and is denoted by the lowest spiro locant.

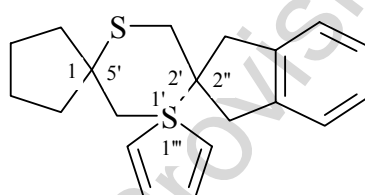
Example:



$2\lambda^6$ -dispiro[bis(1,3,2-benzodioxathiole)-2,1'':2',1''-thiopyran-4'',1'''-cyclopentane] (PIN)

When there is a choice for locants, the lowest set of locants for all spiro atoms is selected, first by comparing them as a set in increasing numerical order, and, if still undecided, in the order of citation in the name. If a choice still remains, criteria involving the heteroatoms and indicated hydrogen atoms are taken into consideration (see Section P-3.2 in ref. 8)

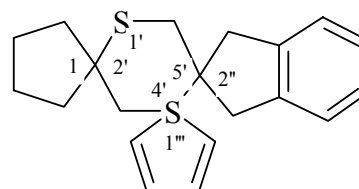
Examples:



(I)

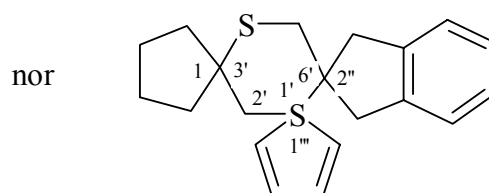
correct

not



(II)

incorrect



incorrect

$1'\lambda^4$ -trispiro[cyclopentane-1,5'-[1,4]dithiane-2',2''-indane-1',1'''-thiophene] (I) (PIN)
[not $4'\lambda^4$ -trispiro[cyclopentane-1,2'-[1,4]dithiane-5',2''-indane-4',1'''-thiophene] (II);
nor $1'\lambda^4$ -trispiro[cyclopentane-1,3'-[1,4]dithiane-6',2''-indane-1',1'''-thiophene] (III);
the locant set '1,1',1''',2',2'',5' ' in (I) is lower than '1,1''',2',2'',4',5' ' in (II), or
'1,1',1''',2'',3',6' ' in (III)]