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EXTENSION AND REVISION OF THE NOMENCLATURE FOR SPIRO COMPOUNDS

(IUPAC Recommendations 1999)

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Extension and revision of the nomenclature for spiro compounds (IUPAC Recommendations 1999)

Abstract: Spiro ring systems have two or more rings linked by one common atom. Several different methods are used to name such systems. Rules A-41, A-43, B-10 and B-12 (Nomenclature of Organic Chemistry, 1979) describe the basics of how to name these compounds. The alternative methods in rules A-42 and B-11 are abandoned.

This document describes the nomenclature in greater detail and extends it to cover branched polyspiro systems and compounds where three rings have one common spiro atom. A new notation, based on the von Baeyer method of naming spiro systems where all components are monocyclic, allows both unbranched and branched polyspiro systems to be named without ambiguity. It also enables the names to be readily interpreted.

PREAMBLE

The nomenclature and name spirane were proposed by von Baeyer [1] for bicyclic compounds with only one atom common to both rings. When a polycyclic ring system is spiro-fused to another ring or ring system Radulescu [2] recognised that each ring system needed to be named separately and, in addition, details of the spiro-fusion must be specified. These two systems were adopted by Patterson [3] in his study of ring systems. A third method of naming spiro compounds was adopted by The Chemical Society [4], which was documented with the other two in the IUPAC rules [5]. The von Baeyer system was covered by rules A-41.1 to A-41.3, A-43.1, B-10.1, and B-12.1; see also C-331.2, C-514.3, D-6.24, D-6.93 and D-7.51 for further examples. Its extension to three or more monocyclic rings spiro-fused is in rule A-41.6. The method for systems containing polycyclic components is in rules A-41.4, A-41.7, A-43.1, B-10.2 and B-12.1 and the third method, which is not used in this document, is in rules A-42 and B-11.1. A special method used when both polycyclic systems are identical is in rule A-41.5, B-10.2, D-6.71 and D-6.94. See also the summary in recommendation R-2.4.3 [6]. Additional examples are given in the Radicals, Ions and Radical Ions document [7].

In this document only the von Baeyer system, the spirobi[....] and spiro[....] methods are documented and extended to more complex systems, for example with branched spiro systems. In most cases the methods closely follow *Chemical Abstracts* practice ([8], Appendix IV, ¶ 156). Some differences are noted below.

This document replaces rules A-41, A-43, B-10, B-12 and R-2.4.3. The alternative methods of rules A-42 and B-11 are abandoned.

SP-0 Spiro

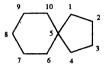
A spiro compound has two (or three) rings which have only one atom in common and the two (or three) rings are not linked by a bridge. The rings may form part of other ring systems (fused ring, bridged fused ring, system named by von Baeyer nomenclature, etc.). The common atom is known as a spiro atom. Spiro-fusion has been termed spiro union.

SP-1 Compounds with only monocyclic ring components

SP-1.1 Monospiro hydrocarbons with two monocyclic rings are named by the prefix spiro before a von Baeyer descriptor (indicating the numbers of carbon atoms linked to the spiro atom in each ring in ascending order and separated by a full stop) placed in square brackets and then the name of the parent hydrocarbon indicating the total number of skeletal atoms, e.g. spiro[4.4]nonane.

SP-1.2 Monospiro hydrocarbons with two monocyclic rings are numbered consecutively starting in the smaller ring at an atom next to the spiro atom, proceeding around the smaller ring back to the spiro atom and then round the second ring.

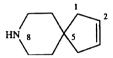
Example:



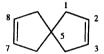
spiro[4.5]decane not spiro[5.4]decane

SP-1.3 Heteroatoms are indicated by replacement prefixes (rules B-4.2, B-6.1, [5]; and rules R-1.2.2.1 and R-9.3, [6]) and unsaturation is indicated in the usual way (rule A-11.3, [5]; R-3.1.1, [6]) by the endings ene, diene, etc.

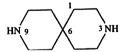
Examples:



8-azaspiro[4.5]dec-2-ene



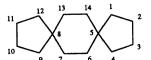
spiro[4.4]nona-2,7-diene



3,9-diazaspiro[5.5]undecane

SP-1.4 Unbranched polyspiro hydrocarbons composed of only monocyclic rings are named using dispiro-, trispiro-, etc. indicating the total number of spiro atoms present and the name of the parent hydrocarbon corresponding to the total number of carbon atoms present. Between the prefix and hydrocarbon name there is placed the von Baeyer descriptor which indicates the number of carbon atoms linked to the spiro atom or linking spiro atoms. The numbers are cited in order starting with a terminal ring and proceeding to the other terminal ring and back to the first via the other linking units. The numbers are separated by full stops and placed in square brackets. The compound is numbered in the order in which the numbers of its von Baeyer descriptor are cited. For trispiro and higher spiro systems each time a spiro atom is reached for the second time its locant is cited as a superscript number to the corresponding number of linking atoms [9].

Examples:

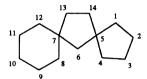


dispiro[4.2.4.2]tetradecane

trispiro[2.2.2.2⁹.2⁶.2³]pentadecane

Note: In previous rules [5,6] superscript numbers were not used but with the extension of this system to branched spiro systems (see SP-1.5) where superscript numbers are essential it is clearer to use them for all polyspiro systems with three or more spiro atoms using a von Baeyer descriptor.

SP-1.4.1: If there is a choice of numbers the name that gives the lower locants for spiro atoms is selected. Example:



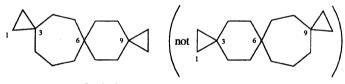
dispiro[4.1.5.2]tetradecane

not dispiro[5.1.4.2]tetradecane nor dispiro[4.2.5.1]tetradecane nor dispiro[5.2.4.1]tetradecane

(5,7 is lower than 6,8 or 5,8 or 6,9)

SP-1.4.2: If there is still a choice of numbering the numbers of the von Baeyer descriptor are considered in the order of citation. The name is selected with lower numbers at the first point of difference.

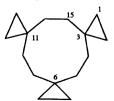
Example:



trispiro[$2.2.2.2^9.2^6.3^3$]hexadecane not trispiro[$2.2.2.2^9.3^6.2^3$]hexadecane ($2.2.2.2^9.2^6.3^3$ is lower than $2.2.2.2^9.3^6.2^3$)

SP-1.5 Branched polyspiro hydrocarbons composed of only monocyclic rings are named using trispiro-, tetraspiro-, etc. indicating the total number of spiro atoms present and the name of the parent hydrocarbon corresponding to the total number of carbon atoms present. Between the prefix and hydrocarbon name there is placed the von Baeyer descriptor which indicates the number of carbon atoms linked to the spiro atom or linking spiro atoms. The numbers are cited in order starting with a terminal ring and proceeding to the next terminal ring and so on to the first spiro atom. The numbers are separated by full stops and placed in square brackets. The compound is numbered in the order in which its von Baeyer descriptor is cited. Each time a spiro atom is reached for the second time its locant is cited as a superscript number to the corresponding number of linking atoms [9].

Examples:

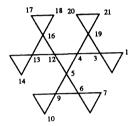


trispiro[2.2.2⁶.2.2¹¹.2³]pentadecane

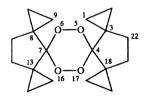
Note: Without the superscript numbers this name would be the same as the name of the second example under SP-1.4 without superscript numbers.

tetraspiro[5.1.5⁸.1.5¹⁵.1.5²².1⁶]dodecasiloxane

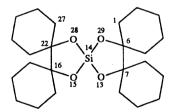
CAS index name does not have the superscript numbers. Without superscript numbers more than one structure is possible.



nonaspiro $[2.0.0.0.2^6.0.2^9.0^5.0.0.2^{13}.0.2^{16}.0^{12}.0^4.0.2^{19}.0^3]$ henicosane



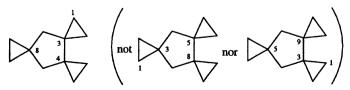
5,6,16,17-tetraoxahexaspiro[2.0.2.0.2⁸.2.2¹³.0⁷.2⁴.0.2¹⁸.2³]docosane



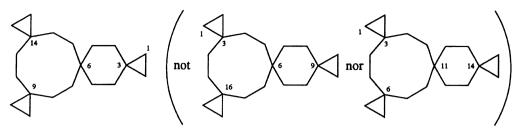
13,15,28,29-tetraoxa-14-silapentaspiro[5.0.5⁷.1.1.5¹⁶.0.5²².1¹⁴.1⁶]nonacosane

SP-1.5.1 If there is a choice of numbering the name which gives the lowest locants for spiro atoms is selected.

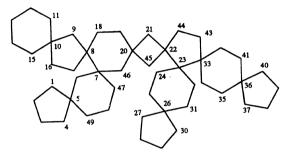
Examples:



trispiro[$2.0.2^4.1.2^8.1^3$]undecane not trispiro[$2.1.2^5.0.2^8.1^3$]undecane nor trispiro[$1.2.2^5.1.2^9.0^3$]undecane (3,4,8 is lower than 3,5,8 or 3,5,9)



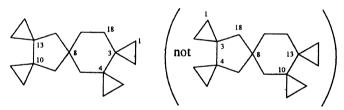
tetraspiro[$2.2.2.2^9.2.2^{14}.2^6.2^3$]icosane not tetraspiro[$2.2.2.2^9.2^6.2.2^{16}.2^3$]icosane nor tetraspiro[$2.2.2^6.2.2.2^{14}.2^{11}.2^3$]icosane (3,6,9,14 is lower than 3,6,9,16 or 3,6,11,14)



decaspiro[4,1.0.1.5 10 .2 8 .2.1.0.2.4 26 .2 23 .0.2.4 36 .2 33 .2 22 .1 20 .1 7 .3 5]nonatetracontane Ref 10 name decaspiro[$\bar{4}$.1.0(1. $\bar{5}$.2)2.1.0(2. $\bar{4}$.2)0.2. $\bar{4}$.2.1.1.3]nonatetracontane

SP-1.5.2 If there is still a choice of numbering the numbers of the von Baeyer descriptor are considered in the order of citation. The name is selected with lower numbers at the first point of difference.

Example:



pentaspiro[$2.0.2^4.1.1.2^{10}.0.2^{13}.1^8.2^3$]octadecane not pentaspiro[$2.0.2^4.1.1.2^{10}.0.2^{13}.2^8.1^3$]octadecane ($2.0.2^4.1.1.2^{10}.0.2^{13}.1^8.2^3$ is lower than $2.0.2^4.1.1.2^{10}.0.2^{13}.2^8.1^3$)

SP-1.6 Ring systems composed of three monocyclic rings with only one spiro atom (i.e. a hexavalent spiro atom) are named by placing the prefix spiro- before the von Baeyer descriptor followed by the name corresponding to the hydrocarbon with the total number of skeletal atoms present in the ring system. Heteroatoms are indicated by replacement terms (SP-1.3) and non-standard valency by the lambda symbol [11] (see SP-7 for further details). The locant of the spiro atom is used as a superscript number to the corresponding number of the von Baeyer descriptor to indicate each time the spiro atom is revisited [9].

Example:



1,4,6,9,10,13-hexaoxa- $5\lambda^6$ -thiaspiro $[4.4^5.4^5]$ tridecane

SP-1.6.1 If there is a choice a smaller ring is numbered before a larger ring.

Example:

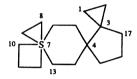


 $3\lambda^6$ -thiaspiro[2.4³.5³]dodecane

SP-1.7 Polyspiro systems which include three rings with a single spiro atom and are composed of monocyclic rings are named using a combination of sections SP-1.4, SP-1.5 and SP-1.6. If there is a choice of numbering the following criteria are considered in order.

SP-1.7.1 Low numbers are selected for spiro atoms

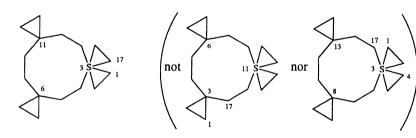
Example:



 $7\lambda^6$ -thiatrispiro[2.0.2.2⁷.3⁷.2⁴.3³]heptadecane

SP-1.7.2 Low numbers are selected for spiro atoms connecting three rings.

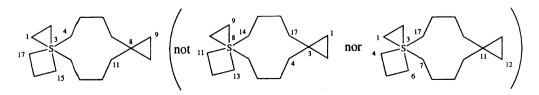
Examples:



 $3\lambda^6$ -thiatrispiro[2.2.2 6 .2.2 1 .2 3 .2 3]heptadecane

not $11\lambda^6$ -thiatrispiro[2.2.2⁶.2.2¹¹.2¹¹.2³]heptadecane (3 is lower than 11)

nor $3\lambda^6$ -thiatrispiro[2.2³.2.2⁸.2.2¹³.2³]heptadecane (3,6,11 is lower than 3,8,13, see SP-1.7.1)



 $3\lambda^6$ -thiatrispiro[2.4.2⁸.4³.3³]heptadecane

not $8\lambda^6$ -thiadispiro[2.4.2⁸.3⁸.4³]heptadecane (3 is lower than 8)

nor 3\delta^6-thiadispiro[2.3\delta.4.2^{11}.4\delta]heptadecane (3,8 is lower than 3,11, see SP-1.7.1)

SP-1.7.3 Low numbers are selected for the von Baeyer descriptor in the order of citation.

Example:

$$\begin{array}{c|c}
14 & 10 \\
\hline
3 & 5 & 7 \\
\hline
11 & 7 & 8
\end{array}$$

$$\begin{array}{c|c}
10 & 14 & 1 \\
\hline
7 & 5 & 3 \\
\hline
12 & 12 \\
\hline
\end{array}$$

 $5\lambda^6$ -thiatrispiro[2.1.1.2⁷.1⁵.2⁵.2³]tetradecane

not $5\lambda^6$ -thiatrispiro[$2.1.1.2^7.2^5.2^5.1^3$]tetradecane

 $(2.1.1.2^7.1^5.2^5.2^3$ is lower than $2.1.1.2^7.2^5.2^5.1^3$)

SP-1.8 If there is a choice of names or numbering due to heteroatoms, functional groups or substituents the following criteria are considered in order until a decision is made:

SP-1.8.1 Low locants are allocated for heteroatoms indicated by replacement terms as a set.

Examples:



1-oxaspiro[4.5]decane

not 4-oxaspiro[4.5]decane



9-oxa-6-azaspiro[4.5]decane

not 7-oxa-10-azaspiro[4.5]decane (6,9 is lower than 7,10)

SP-1.8.2 Low locants are allocated for heteroatoms in the order of B-1.1 [5], RB-1.4 [12], R-2.3.3.1 and R-9.3 [6].

Example:



6-oxa-10-azaspiro[4.5]decane

not 10-oxa-6-azaspiro[4.5]decane (6-oxa is lower than 10-oxa)

SP-1.8.3 Low locants are allocated for non-standard valency indicated by the λ symbol [11], if necessary in order of decreasing numerical value of the bonding number, i.e. the lower number is assigned to λ^5 rather than λ^3 . (See also SP-7.)

Example:



 $6\lambda^5$, 10-diphosphaspiro [4.5] decane

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SP-1.8.4 Low locants are allocated for radical positions, or, if the ring system is a substituent, its point of attachment.

Examples:



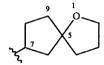
spiro[4.5]decan-2yl

not spiro[4.5]decan-3-yl



3,9-diazaspiro[5.5]undecan-9-ium-3-yl

not 3,9-diazaspiro[5.5]undecan-3-ium-9-yl



However 1-oxaspiro[4.4]nonan-7-yl

not 6-oxaspiro[4.4]nonan-2-yl (see SP-1.8.1)

SP-1.8.5 Low locants are allocated for cationic sites. (See SP-8 for compounds with ionic spiro atoms.)

Example:

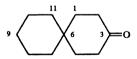


6,6-dimethyl-6,10-diazaspiro[4.5]decan-6-ium (preferred name)

Alternative name 6,6-dimethyl-10-aza-6-azoniaspiro[4.5]decane not 10,10-dimethyl-6,10-diazaspiro[4.5]decan-10-ium (6-ium is lower than 10-ium)

SP-1.8.6 Low locants are allocated for the principal functional group.

Example:

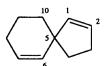


spiro[5.5]undecan-3-one

not spiro[5.5]undecan-9-one (3 is lower than 9)

SP-1.8.7 Low locants are allocated for double bonds.

Examples:



spiro[4.5]deca-1,6-diene

not spiro[4.5]deca-1,9-diene (1,6 is lower than 1,9)

However spiro[4.5]deca-1,9-dien-6-one

not spiro[4.5]deca-1,6-dien-10-one (6-one is lower than 10-one, SP-1.8.6)

SP-1.8.8 Low locants are allocated for substituents cited as prefixes regardless of kind.

Example:

1,1,8,8,12,12-hexamethyldispiro[4.1.4.2]tridecane

not 1,1,8,8,13,13-hexamethyldispiro[4.1.4.2]tridecane

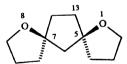
SP-1.8.9 Low locants are allocated for substituents cited as prefixes in the order of citation.

Example:



6,6-diethyl-9,9-dimethyl-1-oxaspiro[4.4]nonane

SP-1.8.10 Low locants are allocated for chirality centres that have the configuration *R*. (See also SP-9.) Example:



(5R,7S)-1,8-dioxadispiro[4.1.4.2]tridecane

not (5S,7R)-1,8-dioxadispiro[4.1.4.2]tridecane (5R is lower than 5S)

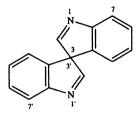
SP-2 Monospiro compounds containing two identical polycyclic components

SP-2.1 Monospiro compounds containing two identical polycyclic components (ignoring double bonds and heteroatoms with a component named by von Baeyer nomenclature) are named by placing the prefix spirobi- before the name of the component ring system in square brackets. Locants required to define the component ring system are placed in square brackets. The established numbering system of the polycyclic component system is retained with one set primed. The location of the spiro atom is indicated in the name by the appropriate locants (unprimed first) placed in front of the name. If there is a choice lower numbers are selected. Where appropriate the system is made mancude [13] after construction of the whole skeleton. If indicated hydrogen is needed to locate double bonds this is cited in front of the spiro atom locants. If there is a choice lower numbers are selected for indicated hydrogen.

Examples:

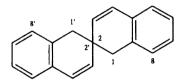
1,1'-spirobi[indene]

CAS index name 1,1'-spirobi[1H-indene]



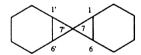
3,3'-spirobi[indole]

CAS index name 3,3'-spirobi[3H-indole]



1*H*,1'*H*-2,2'-spirobi[naphthalene]

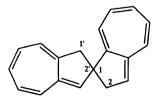
CAS index name 2,2'(1H,1'H)-spirobinaphthalene



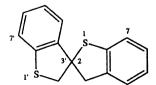
7,7'-spirobi[bicyclo[4.1.0]heptane]

SP-2.2 If there is a choice of which component has primed locants, the lower number at the spiro atom is unprimed.

Examples:



1'H,2H-1,2'-spirobi[azulene]



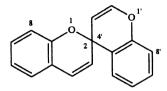
2'H,3H-2,3'-spirobi[[1]benzothiophene]

CAS index name 2,3'(2'H,3H)-spirobi[benzo[b]thiophene]

Note: The indicated hydrogen at 2' may be omitted.

4H-2,4'-spirobi[[1,3]dioxolo[4,5-c]pyran]

CAS index name 2,4'-spirobi[4H-1,3-dioxolo[4,5-c]pyran]

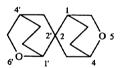


2,4'-spirobi[chromene]

CAS index name spiro[2*H*-1-benzopyran-2,4'-[4*H*-1]benzopyran]

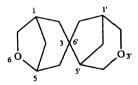
SP-2.3 With components named by von Baeyer nomenclature heteroatoms are indicated by replacement nomenclature. The spiro system is named as the saturated hydrocarbon with replacement term prefixes in front of the completed spiro hydrocarbon name to indicate the heteroatoms. If there is a choice, low numbers are given to the spiro atom then to the heteroatoms. (See SP-1.8 for a more detailed treatment.)

Examples:



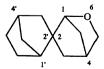
5,6'-dioxa-2,2'-spirobi[bicyclo[2.2.2]octane]

not 6,8'-dioxa-2,2'-spirobi[bicyclo[2.2.2]octane] (5,6'-dioxa is lower than 6,8'-dioxa)



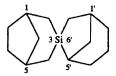
3',6-dioxa-3,6'-spirobi[bicyclo[3.2.1]octane]

CAS index name spiro[3-oxabicyclo[3.2.1]octane-6,3'-[6]oxabicyclo[3.2.1]octane]



6-oxa-2,2'-spirobi[bicyclo[2.2.1]heptane]

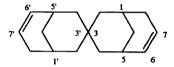
CAS index name spiro[bicyclo[2.2.1]heptane-2,2'-[6]oxabicyclo[2.2.1]heptane]



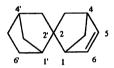
3-sila-3,6'-spirobi[bicyclo[3.2.1]octane

SP-2.4 Unsaturation in a component named by von Baeyer nomenclature is indicated by the endings -ene, -diene, etc.; only the final 'e' of the saturated hydrocarbon name is elided if followed by a vowel. If there is a choice low numbers are given to: (i) spiro atoms, then (ii) replacement terms, (iii) principal functional groups, (iv) double bonds.

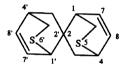
Examples:



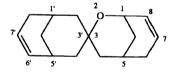
3,3'-spirobi[bicyclo[3.3.1]nonane]-6,6'-diene



2,2'-spirobi[bicyclo[2.2.1]heptan]-5-ene



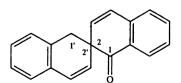
5,6'-dithia-2,2'-spirobi[bicyclo[2.2.2]octane]-7,7'-diene



2-oxa-3,3'-spirobi[bicyclo[3.3.1]nonane]-6',7-diene

SP-2.5 If a choice for the numbering of the components remains, the normal rules for numbering the components are applied; unprimed locants are selected in preference to identical locants with a prime. (See SP-1.8 for a more detailed treatment. If the choice involves indicated hydrogen it should be considered between SP-1.8.5 and SP-1.8.6.)

Examples:



1H,1'H-2,2'-spirobi[naphthalen]-1-one

Note: The 1*H* may be omitted.

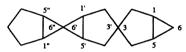
2,2'-spirobi[bicyclo[2.2.2]octane]-5',7-dien-6-one

note 2,2'-spirobi[bicyclo[2.2.2]octane]-5,7'-dien-6'-one

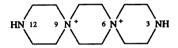
SP-3 Three identical components spiro-fused together

SP-3.1 Dispiro compounds where each component is identical are named by placing the prefix dispiroter-before the name of the component ring system in square brackets. Locants required to define the component ring system are placed in square brackets. The middle component is numbered with primed locants and the numbers of the third component are 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]



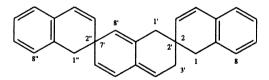
However $3.6\lambda^5.9\lambda^5.12$ -tetraazadispiro[5.2.5.2]hexadecane-6,9-bis(ylium)

(see SP-8 for naming of compounds with ionic spiro atoms)

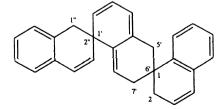
Note This ring system has been called *N*,*N* "-dispirotripiperazinium.

SP-3.2 If there is a choice of locants the lowest set of locants for all spiro atoms is selected when compared as a set in ascending order and, if still undecided, in citation order. If a choice still remains the criteria of SP-1.8 apply. Indicated hydrogen is considered between SP-1.8.5 and SP-1.8.6.

Examples:



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



1''H,2H,5'H,7'H-1,6':1',2''-dispiroter[naphthalene]

not 1'H,1''H,2H,3'H-1,2':5',2''-dispiroter[naphthalene] nor 1H,2''H,5'H,7'H-2,1':6',1''-dispiroter[naphthalene]

(1,1',2'',6') is lower than 1,2',2'',5' or 1',1'',2,6'

1'H, 1''H, 2H, 8'H-1, 2': 7'2''-dispiroter[naphthalen]-1'-one

SP-3.3 Ring systems composed of three identical components with only one spiro atom are named by placing the prefix spiroter- before the name of the component ring system in square brackets. The three spiro locants are indicated in front of the name.

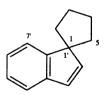
Example:

 $2\lambda^6, 2', 2''$ -spiroter[[1,3,2]benzodioxathiole] (see SP-7 for the use of λ)

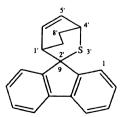
SP-4 Monospiro compounds with different components at least one of which is polycyclic

SP-4.1 Monospiro compounds with different components at least one of which is polycyclic are named by placing the component names within square brackets in alphabetical order and prefixing this with spiro. The position of the spiro atom is denoted by the appropriate locants separated by a comma placed between the two component names. Locants of the second component are primed and any locants needed to name this component ring system are not primed but placed in square brackets. Indicated hydrogen is cited if necessary in front of the complete name.

Examples:



spiro[cyclopentane-1,1'-indene]



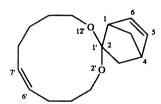
spiro[fluorene-9,2'-[3]thiabicyclo[2.2.2]oct[5]ene] CAS index name spiro[9*H*-fluorene-9,3'-[2]thiabicyclo[2.2.2]oct[5]ene]

1'*H*-spiro[imidazolidine-4,2'-quinoxaline]

spiro[piperidine-4,9'-xanthene]

4',7'-dihydrospiro[1,3-dioxolane-2,2'-[4,7]epoxyindene]

3*H*-spiro[1-benzofuran-2,1'-cyclohex[2]ene]



spiro[bicyclo[2.2.1[hept-5-ene-2,1'-[2,12]dioxacyclododec[6]ene]

SP-4.2 If alphabetical order is inadequate to decide between two names ring seniority principles based on lower italic fusion letters and numbers, heteroatom locants and von Baeyer cypher are used (see C-14.11, [5]).

Examples:

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

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

SP-4.3 Ring systems composed of three components, at least two of which are different, and with only one spiro atom are named by placing the prefix spiro in front of the names of the components in alphabetical order with the appropriate spiro locants. The multiplicative prefix bis- is used for identical components. With three different components the component cited in the middle of the name is enclosed in parentheses to highlight this unusual situation. (See SP-7 for the use of λ .)

Examples:

 $2\lambda^6$ -spiro[1,3,2-benzodioxathiole-2,2'-([1,2,3]benzoxadithiole)-2.5"-dibenzo[b,d]thiophene]

 $2\lambda^6$ -spiro[bis([1,3,2]benzodioxathiole)-2,2':2,2"-[1,2,3]benzoxadithiole]

SP-4.4 Ring systems spiro-fused to natural products may also be named in a similar way to SP-4.1. Examples are steroids (rule 3S-10.3, [14]) and carbohydrates (rule 2-Carb-35.3, [15]).

SP-5 Unbranched polyspiro compounds with at least two different components and at least one of which is polycyclic

SP-5.1 Unbranched polyspiro compounds with at least two different components and at least one of which is polycyclic are named by placing each component name in order of occurrence in square brackets beginning with the terminal component earlier in alphabetical order, with a prefix to indicate the number of spiro atoms in front (dispiro-, trispiro-, etc.). Locants of the first cited component are unprimed, the next one is primed and so on. Locants which form part of the name of the second and later components are not primed but cited in square brackets. The positions of the spiro atoms are indicated by the appropriate pair of locants separated by a comma between each pair of component ring system names. Indicated hydrogen, if necessary, is cited in front of the complete name. If there is a choice of names the first cited is the one earlier in alphabetical order for the second (then third etc.)

component. Multiplicative prefixes are not used with dispiro systems having identical terminal components.

Examples:

dispiro[fluorene-9,1'-cyclohex[2]ene-4',1"-indene]

not dispiro[indene-1,1'-cyclohex[2]ene-4',9"-fluorene] [fluorene before indene]

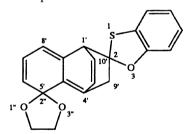
2"H,4"H-trispiro[cyclohexane-1,1'-cyclopentane-3',3"-cyclopenta[b]pyran-6",1""-cyclohexane]

not 2'H,4'H-trispiro[cyclohexane-1,6'-cyclopenta[b]pyran-3',1"-cyclopentane-3",1"-cyclohexane]

[cyclopentane before cyclopenta[b]pyran]

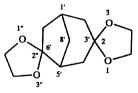
Note that the 2''H is not strictly necessary here.

SP-5.2 If there is a choice of locants the criteria of SP-3.2 and then SP-1.8 apply until a decision is made. Examples:



1'H-dispiro[1,3-benzoxathiole-2,10'-[1,4]ethanonaphthalene-5',2"-[1,3]dioxolane]

not 4'H-dispiro[1,3-benzoxathiole-2,9'-[1,4]ethanonaphthalene-8',2"-[1,3]dioxolane] (2,2",5',10' is lower than 2,2",8',9')



dispiro[1,3-dioxolane-2,3'-bicyclo[3.2.1]octane-6',2"-[1,3]dioxolane]

not dispiro[1,3-dioxolane-2,6'-bicyclo[3.2.1]octane-3',2''-[1,3]dioxolane] [2,3',6',2'' is lower than 2,6',3',2'']

nor dispiro[bicyclo[3.2.1]octane-3,2':6,2"-bis([1,3]dioxolane)]

Note: This is the traditional method of naming such systems but the use of a multiplicative prefix as in the third name of the above example is more concise and unambiguous.

SP-6 Branched polyspiro compounds with at least one polycyclic component

When three or more components are spiro-fused to the same component the ring system is described as a branched spiro-fused ring system. Terminal components have only one spiro atom.

SP-6.1 If a central component is spiro-fused 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 are primed, double primed etc. The spiro atoms are indicated by pairs of locants separated by colons. Indicated hydrogen is cited if necessary in front of the complete name.

Example:

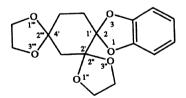
trispiro[1,3,5-trithiane-2,2':4,2'':6,2'''-tris(bicyclo[2.2.1]heptane)]

SP-6.2 If two or more different terminal components are spiro-fused to a central component the alphabetically first is quoted first with a multiplicative prefix if appropriate followed by the central component and then the remaining terminal components in alphabetical order.

Examples:

trispiro[adamantane-2,3'-[1,2,4,5,7,8]hexoxonane-6',1":9',1""-bis(cyclohexane)] (preferred name) Alternative name

transpiro[bis(cyclohexane)-1,3":1',6"-[1,2,4,5,7,8]hexoxonane-9",2""-tricyclo[3.3.1.1^{3,7}]decane]



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

 $2\lambda^6\text{-dispiro[bis}([1,3,2]benzodioxathiole)-2,1^{\prime\prime}:2^\prime,1^{\prime\prime}\text{-thiopyran-4}^{\prime\prime},1^{\prime\prime\prime}\text{-cyclopentane}]$

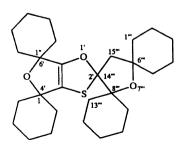
trispiro[cyclopentane-1,1'-cyclohexane-3',2"-imidazole-5',1"'-indene]

SP-6.3 If there is a choice of locants the criteria of SP-3.2 and then SP-1.8 apply. Example:

 $1'\lambda^4\text{-trispiro[cyclopentane-1,5'-[1,4]dithiane-2',2''-indane-1',1'''-thiophene]} \\ \text{not } 1'\lambda^4\text{-trispiro[cyclopentane-1,3'-[1,4]dithiane-6',2''-indane-1',1'''-thiophene]} \\ \text{nor } 4'\lambda^4\text{-trispiro[cyclopentane-1,2'-[1,4]dithiane-5',2''-indane-4',1'''-thiophene]} \\ (1,1',1''',2',2'',5' \text{ is lower than } 1,1',1''',2'',3',6' \text{ or } 1,1''',2',2'',4',5')} \\$

- **SP-6.4** If additional components are spiro-fused to a branched polyspiro compound as described in SP-6.1 to SP-6.3 the following criteria are applied in order:
- (a) Any monocyclic ring components spiro-fused together are named (see SP-1) as a unit containing the maximum number of monocyclic ring components. This unit is used as a component for further spiro-fusion (see SP-5). To help indicate the composite nature of the name braces are used (instead of square brackets) after the initial polyspiro prefix to enclose components at least one of which is already spiro-fused.
- (b) If there is not a polyspiro system composed of monocyclic ring components or the system cannot be named by the normal spiro-fusion rules (see SP-2 to SP-6.1) the largest preferred spiro system is named and treated as a unit for further spiro-fusion. The priming of this unit is continued in the rest of the name.
- **SP-6.4.1** After identification of the spiro-fused components these, together with the remaining components, are treated in the normal way. For example SP-5 or SP-6.2 may apply.

Examples:



trispiro{bis(cyclohexane)-1,4':1'',6'-furo[3,4-d][1,3]oxathiole-2',14'''-[7]oxadispiro-[5,1,5.2]pentadecane} CAS index name

pentaspiro[tetracyclohexane-1,2'(5'H):1''',5':1'''',4''(6''H):1''''',6''-furan-3'(4'H),2''-furo[3,4-d][1,3]oxathiole]

 $trispiro\{1-oxaspiro[2.3] hexane-2, 3':4, 3'':5, 3'''-tris(tetracyclo[3.2.0.0^{2,7}.0^{4,6}] heptane]\}$

Note: There are only two monocyclic rings spiro-fused together.

 $1\lambda^5, 3\lambda^5, 5\lambda^5, 7\lambda^5 - tetraspiro\{tetraspiro[2,4,6,8,9,10-hexathia-1,3,5,7-tetraphosphaadamantane-1,2':3,2'':5,2''':7,2''''-tetrakis([1,3,2]oxathiaphosphetane)]-4',7''''':4'',7'''''':4''',7'''''':4'''',7''''''-tetrakis(pyrano[2,3-c]acridine)\} [criterion SP-6.4 (d)]
CAS index name octaspiro[2,4,6,8,9,10-hexathia-1,3,5,7-tetraphosphatricyclo[3.3.1.1^{3,7}]decane-1,2'<math>\lambda^5$:3,2" λ^5 :5,2"' λ^5 :

 $7,2^{\prime\prime\prime\prime}\lambda^5$ -tetrakis[1,3,2]oxathiaphosphetane- $4^\prime,7^{\prime\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime}:4^{\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime}:4^{\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime}:4^{\prime\prime\prime}:4^{\prime\prime\prime},7^{\prime\prime\prime}:4^{\prime\prime\prime}:4^{\prime\prime\prime}:4^{\prime\prime\prime}:4^{\prime\prime\prime}:4^{\prime\prime}:4^{\prime\prime\prime}:4^{\prime\prime}:4$

Note 1: The primes have a space after every four to assist recognition of the number present.

Note 2: See SP-7 for the use of the λ symbol with non-standard valency.

SP-7 Spiro systems containing atoms with non-standard valency

SP-7.1 In addition to the normal use of the lambda symbol [11] there are a number of special situations with spiro systems. Non-standard valency is stated in the normal way with the appropriate locant when cited as part of the name, otherwise at the start of the name. If the spiro atom has non-standard valency the symbol is associated with the less primed locant and is placed at the front of the name except for cases described in SP-7.2. Where there is a choice the first cited component (unprimed locants in a spirobi[....] type name) is used for indicated hydrogen.

Note: CAS index names differ from the above in that the lambda symbol is associated with the more primed locant at a spiro-fusion site and is separately quoted in front of a spirobi[....] type name. As noted below CAS index names do not always name the mancude system [13].

Examples:

 $3H-2\lambda^5$ -spiro[1,3,2-benzoxazaphosphole-2,2'-[1,3,5,2]triazaphosphinine] CAS index name spiro[1,3,2-benzoxazaphosphole-2(3H),2' λ^5 -[1,3,5,2]triazaphosphorine]

2,3-dihydro-1'H-2 λ^5 -spiro[1,3,2-benzoxazaphosphole-2,2'-[1,3,5,2]triazaphosphinine] CAS index name spiro[1,3,2-benzoxazaphosphole-2,2 $'\lambda^5$ (1'H)-[1,3,5,2]triazaphosphorine]

 $1H-2\lambda^5,2'$ -spirobi[[1,3,2]benzodiazaphosphinine]

CAS index name for the 1',2'-dihydro compound is $2\lambda^5-2,2'(1H,1'H)$ -spirobi[1,3,2-benzodiazaphosphorine]

1,5,9,13-tetraoxa-7,14-diaza- $6\lambda^5,8\lambda^5$ -diphosphadispiro[5.1.5.1]tetradecane

 $2\lambda^5$ -spiro[1,3,2-benzodioxaphosphole-2,11'-[1,3,2]oxazaphospholo[3',2':2,3][1,2,4,3]triaza-phospholo [4,5-a]pyridine]

 $1'H, 4'H, 8'H-2\lambda^5$ -spiro[1,3,2-benzodioxaphosphole-2,3a^{2'}-[3a²]phosphadibenzo[cd,mn]pyrene] CAS index name

 $spiro[1,3,2-benzodioxaphosphole-2,13'\lambda^5-[1H,5H,9H]benzo[1,9] phosphinolizino[3,4,5,6,7-defg] acridophosphine]$

Note: The internal number used here follows IUPAC fused ring nomenclature rule FR-5.5.2 [ref 16].

1H, 1'H, 5H, 5'H- $3\lambda^6$, 3'-spirobi[[1,2]oxathiolo[4,3,2-hi][2,1]benzoxathiole]

CAS names this as an octahedral derivative of sulfur

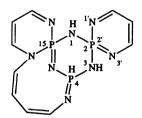
 $3H-2\lambda^5$ -spiro[1,4,2-oxazaphosphole-2,1'-[2,8,9]trioxa[1]phosphaadamantane] (preferred name)

Alternative name

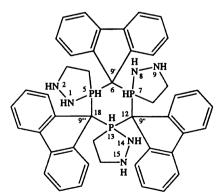
 $3H-2\lambda^5$ -spiro[1,4,2-oxazaphosphole-2,1'-[2,8,9]trioxa[1]phosphatricyclo[3.3.1.1^{3,7}]decane]

SP-7.2 Where the lambda symbol is required to name the component it is cited in the normal way with the component name.

Examples:



 $1H,3H-2\lambda^5$ -spiro[$4\lambda^5,15\lambda^5$ -azeno[1,3,2]diazaphosphinino[1,2-a]-[1,3,5,7,2,4,6]tetraazatriphosphacycloundecine-2,2'-[1,3,2]diazaphosphinine]



trispiro $\{1,2,8,9,14,15$ -hexaaza- $5\lambda^5,7\lambda^5,13\lambda^5$ -triphosphatrispiro $[4.1.4^7,1.4^{13}.1^5]$ octadecane-6,9':12,9'':18,9'''-tris(fluorene) $\}$ (Named using SP-6.4 then SP-6.1)

CAS index name trispiro[1,2,8,9,14,15-hexaaza- $5\lambda^5$, $7\lambda^5$, $13\lambda^5$ -triphosphatrispiro[4.1.4.1.4.1]octadecane-6.9':12.9'':18.9''-tris[9H]fluorene]

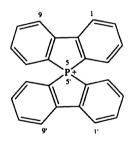
SP-8 Ionic spiro atom

The preferred method for naming spiro compounds with an ionic spiro atom is to indicate a non-standard valency for the spiro atom and generate the ion by the appropriate subtractive or additive suffix [7]. Alternative methods use the ionic replacement terms (see R-5.8.2 and R-5.8.3, [6]) or indicate the ion in the names of the components of the spiro system.

Examples:

 $5\lambda^5$ -arsaspiro[4.4]nonan-5-ylium (preferred name) Alternative name 5-arsoniaspiro[4.4]nonane

 $5\lambda^5$ -phosphaspiro[4.4]nonan-5-uide (preferred name) Alternative name $5\lambda^5$ -phosphanuidaspiro[4.4]nonane



5λ⁵,5'-spirobi[benzo[*b*]phosphindol]-5-ylium (preferred name) Alternative names 9-phosphonia-9,9'-spirobi[fluorene] or 5,5'-spirobi[*b*]phosphinodolium] CAS index name 5,5'-spirobi[5*H*-dibenzophospholinium]



 $5\lambda^7,5',5''$ -spiroter[benzo[b]phosphindol]-5-ide

The parent of this ion was called by CAS 5,5',5''-dispirotri[5H-dibenzophosphole] but is now named as an octahedral complex, tris([1,1'-biphenyl]-2,2'-diyl)phosphate(1-)

1H- $2\lambda^5$ -spiro[isoquinoline-2,2'-pyrido[1,2-a]pyrazin]-2-ylium CAS index name spiro[isoquinoline-2(1H),2'-[2H[pyrido[1,2-a]pyrazinium]

 $2'\textit{H-}3\lambda^5\text{-spiro}[3\text{-azabicyclo}[3.2.2] nonane\text{-}3,3'\text{-}[1,3] oxazol]\text{-}3\text{-ylium}$

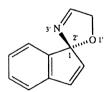
CAS index name spiro[3-azabicyclo[3.2.2]nonane-3,3'(2H)-oxazolium]

Note: 2'H could be omitted.

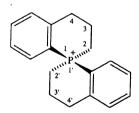
SP-9 Stereochemistry

SP-9.1 Stereochemistry associated with tetrahedral geometry is indicated by the method of section E [5] and R-7 [6] (see also SP-1.8.10). Although most cases are straightforward there are some where Section E is inadequate. (See [17] for a further details.)

Examples:



(R)-5'H-spiro[indene-1,2'-[1,3]oxazole]



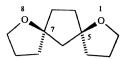
(S)-3,3',4,4'-tetrahydro-2H,2'H-1 λ 5,1'-spirobi[phosphinolin]-1-ylium (preferred name) Alternative name (S)-3,3',4,4'-tetrahydro-2H,2'H-1-phosphonia-1,1'-spirobi[naphthalene]



(S)-1,6-dioxaspiro[4.4]nonane



cis-1,9-dioxadispiro[4.2.4.2]tetradecane



cis-1,8-dioxadispiro[4.1.4.2]tridecane or (5*R*,7*S*)-1,8-dioxadispiro[4.1.4.2]tridecane

 $(5(11)R_a)-1,12$ -dioxatrispiro $[4.2.2.4^{11}.2^8.2^5]$ nonadecane

Note: The stereochemistry is indicated with a compound locant to indicate the chirality axis.

(R)-trispiro $[4.1.1.4^9.2^7.2^5]$ heptadecane

1r,5c,8c,11t-tetraoxatetraspiro[2.0.2⁴.0.2⁷.0.2¹⁰.0³]dodecane

Note: Rules E-2.3.3 [5] and R-7.1.1 [6] would suggest r-1,c-5,c-8,t-11-tetraoxa.... but the *Beilstein* practice [18] is used here as it is shorter and clearer. This change is being considered for the revision of section E (stereochemistry).

SP-9.2 Stereochemistry associated with non-tetrahedral geometry is indicated by the method of coordination chemistry (see I-2.2.3.2, I-10.5 and I-10.7, [19]).

Examples:

 $(TBPY-4-11'-A)-3,3,3',3'-\text{tetramethyl}-3H,3'H-1\lambda^4,1'-\text{spirobi}[[2,1]\text{benzoxathiole}]$

(TPBY-5-11'-A)1-oxo-3,3,3',3'-tetrakis(trifluoromethyl)-3H,3'H-1 λ^6 ,1'-spirobi[[2,1]benzoxathiole] or (TBPY-5,11'-A)-3,3,3',3'-tetrakis(trifluoromethyl)-3H,3'H-1 λ^4 ,1'-spirobi[[2,1]benzoxathiole] 1-oxide

(TBPY-5-12-C)-2-phenoxy- $2\lambda^5$ -spiro[1,3,2-dithiaphosphinane-2,2'-phenanthrol[9,10-d]-[1,3,2] dithiaphosphole]

(SPY-5-21)-2-phenyl-2,2'-spirobi[naphtho[2,3-d][1,3,2]dioxasilol]-2-uide

 $(OC\text{-}6\text{-}12)\text{-}1,1\text{-}difluoro\text{-}3,3,3',3'\text{-}tetrakis(trifluoromethyl)-}3H,3'H\text{-}1\lambda^6,1'\text{-}spirobi[[2,1]benzoxathiole]$

 $(OC\text{-}6\text{-}22\text{-}\Lambda)\text{-}1,1\text{-}difluoro\text{-}1,1\text{-}difluoro\text{-}3,3,3',3'\text{-}tetrakis(trifluoromethyl)-}3H,3'H\text{-}1\lambda^6,1'\text{-}spirobi[[2,1] benzoxathiole]}$

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