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ORGANIC CHEMISTRY DIVISION
COMMISSION ON NOMENCLATURE OF ORGANIC CHEMISTRY (III.1)

EXTENSION AND REVISION OF THE VON BAEYER SYSTEM FOR NAMING POLYCYCLIC COMPOUNDS (INCLUDING BICYCLIC COMPOUNDS)

(IUPAC Recommendations 1999)

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Extension and revision of the von Baeyer system for naming polycyclic compounds (including bicyclic compounds) (IUPAC Recommendations 1999)

Abstract: These recommendations document the von Baeyer system for naming polycyclic ring systems described in Rules A-31, A-32 and B-14 of the *Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F and H,* 1979 and R-2.4.2 of *A Guide to IUPAC Nomenclature of Organic Compounds*, 1993 and extend the system to cover more complex cases. It provides guidance on the naming of ring systems which previously the rules did not cover. The method is to identify the main ring and main bridge which provide the basic bicyclic system and to number these atoms. Then all further bridges, whether or not they include additional atoms, are identified by indicating not only the number of atoms but also the two atoms to which the bridge is attached. The final name also indicates the number of rings and the total number of skeletal atoms in the ring system. Heteroatoms, unsaturation and substituents are indicated in the usual way.

This system of naming polycyclic compounds was first developed for bicyclic compounds by von Baeyer [1] and was extended to tricyclic systems by Buchner & Weigand [2]. Von Baeyer nomenclature was adopted by Patterson [3] in his work for IUPAC on ring nomenclature which was used in the Ring Index [4] and by the Chemical Abstracts Service Index Guide, Appendix IV, ¶ 155, 161, 184 [5]. IUPAC extended von Baeyer nomenclature in the current rules, see rules A-31, A-32 (hydrocarbons), B-14 (heterocyclic compounds) plus examples in B-6.1, C-514.4, C-551.2; see also D-6.24 (siloxanes), D-6.33 (silathianes), D-6.43 (silazanes), D-6.51 (silazane radicals), D-6.71 (organosilicon compounds), D-7.51 (organoboron compounds), and D-7.54 (borazane) [6]. See also a summary in recommendation R-2.4.2 and examples in R-5.8.1.1, R-5.8.1.2, R-5.8.2 and R-7.1.1 [7]; the lambda convention, rule Lm-2.0 [8]; and examples in the radicals and ions document, e.g. RC-81.1.3.3 [9]. Deficiencies in the rules were pointed out by Eckroth [10] and Rücker & Rücker [11]. This document sets out to rectify such deficiencies and replaces the existing rules A-31, A-32 and B-14 [6].

In the examples below the numbering shown refers to the preferred name unless specifically indicated as corresponding to an alternative incorrect name.

Polycyclic ring systems which are to be treated by the von Baeyer system are named by the following rules applied in order until a decision is made.

VB-1 Definitions and terminology

A *bridgehead* is any skeletal atom of the ring system which is bonded to three or more skeletal atoms (excluding hydrogen).

A *bridge* is an unbranched chain of atoms or an atom or a valence bond connecting two bridgeheads.

Two bridgeheads are selected as *main bridgeheads*. These two bridgeheads must be linked by at least three bridges (which may include bridgehead atoms required for secondary bridges). No atom is present in more than one bridge.

The *main ring* of the ring system is the ring identified by VB-2 and includes the two main bridgeheads.

The *main bridge* is a bridge which connects the two main bridgeheads.

A *secondary bridge* is any bridge not included in the main ring or the main bridge.

An *independent secondary bridge* links bridgeheads which are part of the main ring or main bridge.

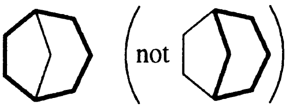
A *dependent secondary bridge* links at least one bridgehead which is part of a secondary bridge.

A *polycyclic system* is regarded as containing a number of rings equal to the minimum number of scissions required to convert the system into an open-chain compound. The number of rings is indicated by the appropriate prefix, bicyclo- (not dicyclo-), tricyclo-, tetracyclo-, etc.

VB-2 Main ring

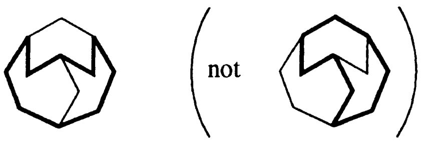
The main ring is selected so as to include as many skeletal atoms of the polycyclic compound as possible. The main ring is shown in bold in examples for VB-2 to VB-4.

Examples



bicyclo[3.2.1]octane

not bicyclo[3.1.2]octane (7-membered main ring larger than 6)



tricyclo[4.4.1.1^{3,9}]dodecane

not tricyclo[4.3.2.1^{3,8}]dodecane (10-membered main ring larger than 9)

VB-3 Naming hydrocarbon bicyclic systems

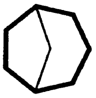
A bicyclic system (which comprises the main ring and main bridge only) is named by:

the prefix bicyclo- (indicating the number of rings);

numbers indicating the bridge lengths (i.e. number of skeletal atoms excluding the bridgehead atoms) separated by full stops and placed in square brackets. The three numbers are cited in decreasing order of size (e.g. [3.2.1]);

the name of the hydrocarbon indicating the total number of skeletal atoms.

Example

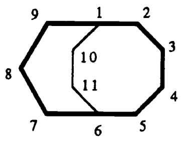


bicyclo[3.2.1]octane

VB-4 Numbering of bicyclic systems

The atoms of a bicyclic system are numbered from a bridgehead atom via the longest path to the second bridgehead atom; numbering of atoms continues round the main ring; and then the main bridge atoms are numbered starting from the lower numbered bridgehead atom.

Example



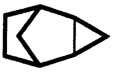
bicyclo[4.3.2]undecane

VB-5 Main bridge

If there is more than one bridge the main bridge is selected to include as many as possible of the atoms not in the main ring.

The main ring and main bridge are shown in bold in examples for VB-5 to VB-7.

Example



tricyclo[3.2.1.0^{2,4}]octane

not tricyclo[4.1.0.1^{2,5}]octane (one-atom main bridge larger than no-atom bridge)

VB-6 Naming hydrocarbon polycyclic systems

Any rings not described by the bicyclic system are defined by citing the number of atoms making up each secondary bridge. The locants of the two attachment points of each secondary bridge are cited as a pair of superscript locants (lower first) separated by a comma. The numbers indicating independent secondary bridges are cited in decreasing order.

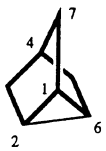
The name of the polycyclic hydrocarbon is then constructed by:

a prefix indicating the number of rings (tricyclo, tetracyclo, etc.);

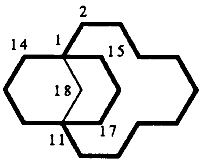
numbers indicating the bridge lengths (with the appropriate superscript locants in the case of secondary bridges) separated by full stops and placed in square brackets (e.g. 4.2.0.0^{2,4}]);

and the name of the parent hydrocarbon indicating the number of ring atoms.

Examples



tricyclo[2.2.1.0^{2,6}]heptane



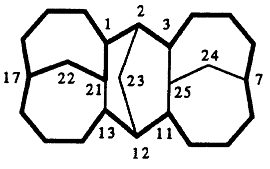
tricyclo[9.3.3.1^{1,11}]octadecane

not tricyclo[9.3.3.1]octadecane

Note: The independent secondary bridge C-18 requires the superscript locants 1,11 to indicate its attachment.

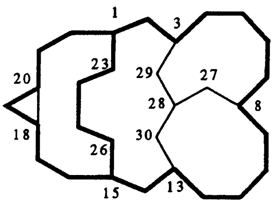
Independent secondary bridges are cited before dependent secondary bridges. The numbers indicating dependent secondary bridges are cited in decreasing order.

Examples



hexacyclo[15.3.2.2^{3,7}.1^{2,12}.0^{13,21}.0^{11,25}]pentacosane

(0^{11,25} is a dependent secondary bridge)



pentacyclo[$13.7.4.3^{3,8}.0^{18,20}.1^{13.28}$]triacontane

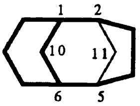
($1^{13.28}$ is a dependent secondary bridge)

Note: The sum of the numbers indicating the atoms in the bridges comprising the main ring, the main bridge and all secondary bridges plus two will equal the number of skeletal atoms present, e.g. in the example above $(13 + 7 + 4 + 3 + 1) + 2 = 30$ hence triacontane.

If there is a choice of names the following criteria are considered in order until a decision is made.

VB-6.1 The main ring shall be divided as symmetrically as possible by the main bridge.

Example

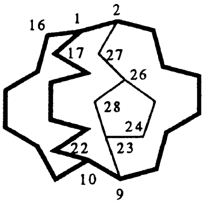


tricyclo[$4.3.1.1^{2,5}$]undecane

not tricyclo[$5.2.1.1^{2,6}$]undecane (4.3 more symmetric than 5.2)

VB-6.2 If there is a choice of independent secondary bridges the first cited shall be as long as possible. Then if relevant the second cited independent secondary bridge shall be as long as possible, etc.

Example

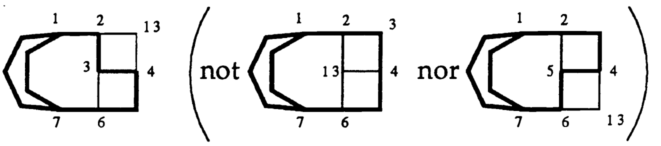


tetracyclo[$8.6.6.5^{2,9}.1^{23,26}$]octacosane

not tetracyclo[$8.6.6.4^{2,9}.2^{23,25}$]octacosane (8.6.6.**5**.1 is higher than 8.6.6.**4**.2)

VB-6.3 The number of dependent secondary bridges is kept to a minimum.

Example



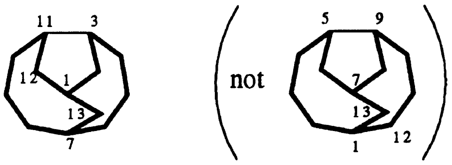
tetracyclo[$5.3.2.1^{2,4}.0^{3,6}$]tridecane

not tetracyclo[$5.3.2.1^{2,4}.0^{6,13}$]tridecane ($0^{6,13}$ is a dependent secondary bridge)

nor tetracyclo[$5.3.2.1^{4,6}.0^{2,5}$]tridecane (see VB-6.4)

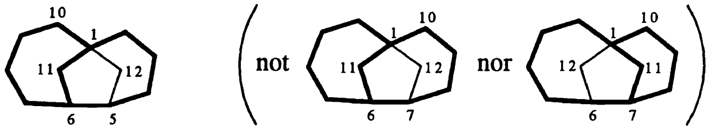
VB-6.4 The superscript locants of the secondary bridges shall be as small as possible when considered as a set in ascending numerical order, a decision being made at the first point of difference.

Examples



tricyclo[5.5.1.$0^{3,11}$]tridecane

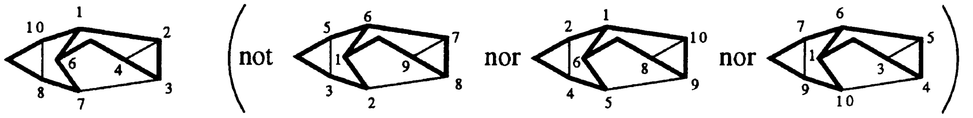
not tricyclo[5.5.1.$0^{5,9}$]tridecane (3,11 is lower than 5,9)



tricyclo[4.4.1.$1^{1,5}$]dodecane

not tricyclo[4.4.1.$1^{1,7}$]dodecane (1,5 is lower than 1,7)

nor tricyclo[5.3.1.$1^{1,6}$]dodecane (4.4 more symmetric division than 5.3 for main ring, see VB-6.1)



pentacyclo[4.4.0.$0^{2,4}$.$0^{3,7}$.$0^{8,10}$]decane

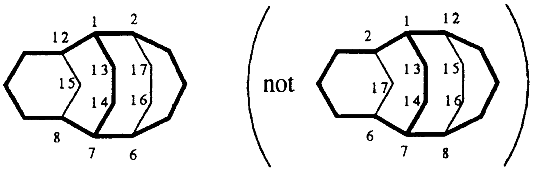
not pentacyclo[4.4.0.$0^{2,8}$.$0^{3,5}$.$0^{7,9}$]decane (2,3,**4**,7,8,10 is lower than 2,3,**5**,7,8,9)

nor pentacyclo[4.4.0.$0^{2,4}$.$0^{5,9}$.$0^{8,10}$]decane (2,**3**,4,7,8,10 is lower than 2,**4**,5,8,9,10)

nor pentacyclo[4.4.0.$0^{3,5}$.$0^{4,10}$.$0^{7,9}$]decane (**2**,3,4,7,8,10 is lower than **3**,4,5,7,9,10)

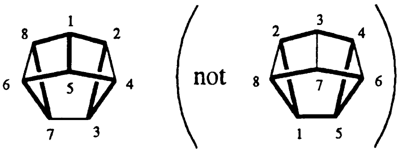
VB-6.5 The superscript locants shall be as small as possible when considered in the order of citation in the name.

Examples



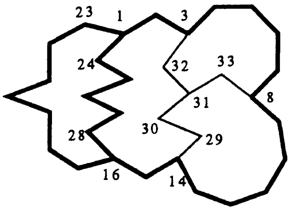
tetracyclo[5.5.2.$2^{2,6}$.$1^{8,12}$]heptadecane

not tetracyclo[5.5.2.$2^{8,12}$.$1^{2,6}$]heptadecane (**2**,6,8,12 is lower than **8**,12,2,6)



entacyclo[3.3.0.$0^{2,4}$.$0^{3,7}$.$0^{6,8}$]octane

not pentacyclo[3.3.0.$0^{2,8}$.$0^{3,7}$.$0^{4,6}$]octane (2,**4**,3,7,6,8 is lower than 2,**8**,3,7,4,6)

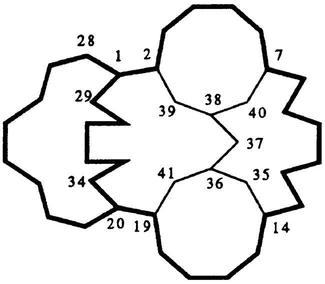


tetracyclo[14.7.5.4^{3,14}.1^{8,31}]tritriacontane

not tetracyclo[14.7.5.4^{8,14}.1^{3,31}]tritriacontane (**3**,14,8,31 is lower than **8**,14,3,31)

nor tetracyclo[14.7.5.4^{3,9}.1^{14,30}]tritriacontane (3,**8**,14,31 is lower than 3,**9**,14,30, see VB-6.4)

nor tetracyclo[14.7.5.4^{3,14}.1^{9,30}]tritriacontane (3,**8**,14,31 is lower than 3,**9**,14,30, see VB-6.4)



pentacyclo[18.8.6.5^{2,14}.1^{7,38}.1^{19,36}]hentetracontane

not pentacyclo[18.8.6.5^{2,19}.1^{7,38}.1^{14,36}]hentetracontane (2,**14**,7,38,19,36 is lower than 2,**19**,7,38,14,36)

nor pentacyclo[18.8.6.5^{7,14}.1^{2,38}.1^{19,36}]hentetracontane (**2**,14,7,38,19,36 is lower than **7**,14,2,38,19,36)

nor pentacyclo[18.8.6.5^{7,19}.1^{2,38}.1^{14,36}]hentetracontane (**2**,14,7,38,19,36 is lower than **7**,19,2,38,14,36)

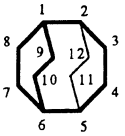
nor pentacyclo[18.8.6.3^{2,7}.3^{14,19}.1^{36,39}]hentetracontane (18.8.6.**5**.1.1 is higher than 18.8.6.**3**.3.1, see VB-6.2)

VB-7 Numbering of secondary bridges

After numbering the main ring and main bridge (see VB-4) all independent secondary bridges are numbered before dependent secondary bridges. The numbering continues from the highest number of the main ring and 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 numbered bridgehead atom and so on. Each atom of a secondary bridge is numbered starting from the atom next to the higher numbered bridgehead.

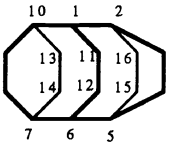
Note: This rule is based on the procedure used by CAS, which is consistent with the method used for the numbering of bridges across fused ring systems (see FR-8.6 and FR-8.7 [12]). The previous version of the rule, A-32.23 [6], has been interpreted in different ways. It is not clear if decreasing order refers to length of bridges or decreasing order of bridgehead locants.

Examples

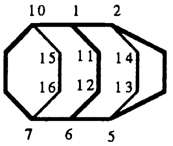


tricyclo[4.2.2.2^{2,5}]dodecane

(the secondary bridge is numbered starting from bridgehead 5)



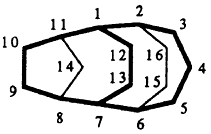
(not



)

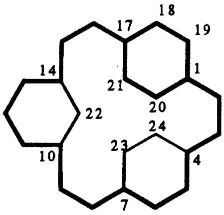
tetracyclo[4.4.2.$2^{2,5}$.$2^{7,10}$]hexadecane

(the first secondary bridge to be numbered is linked to bridgehead 10)



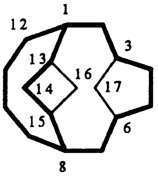
tetracyclo[5.4.2.$2^{2,6}$.$1^{8,11}$]hexadecane

(the first secondary bridge to be numbered is linked to bridgehead 11)



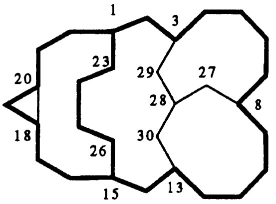
tetracyclo[15.2.2.$2^{4,7}$.$1^{10,14}$]tetracosane

(the first secondary bridge to be numbered is linked to bridgehead 14)



tetracyclo[6.4.3.$1^{3,6}$.$1^{13,15}$]heptadecane

(the first secondary bridge to be numbered is linked to bridgehead 15)

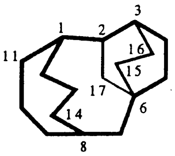


pentacyclo[13.7.4.$3^{3,8}$.$0^{18,20}$.$1^{13,28}$]triacontane

(the independent bridge is numbered before the dependent bridge)

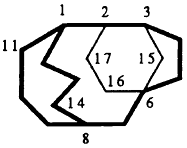
VB-7.1 If there is still a choice lower locants are used for the atoms in the bridge linked to the higher numbered bridgehead.

Examples



tetracyclo[6.3.3.$2^{3,6}$.$1^{2,6}$]heptadecane

(15 and 16 are the bridge to 3 not 2)

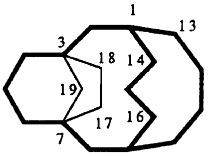


tetracyclo[6.3.3.$2^{2,6}$.$1^{3,6}$]heptadecane

(15 is the bridge to 3 not 2)

VB-7.2 If there is still a choice longer bridges are numbered before shorter bridges.

Example



tetracyclo[7.4.3.$2^{3,7}$.$1^{3,7}$]nonadecane

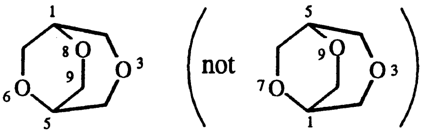
VB-8 Naming modified ring systems (heteroatoms, unsaturation, stereochemistry, etc.)

Heteroatoms are indicated by replacement terms (see B-4.2, B-6.1, R-1.2.2.1, R-9.3); unsaturation is indicated in the usual way by the ending -ene, -diene, etc. (see A-11.3, R-3.1.1); stereochemistry by the *R/S* notation (see E-4.9, R-7.2.1); and substituents and the principal functional group in the usual way [6,7].

If there is still a choice of name or numbering the following criteria are considered in order until a decision is made:

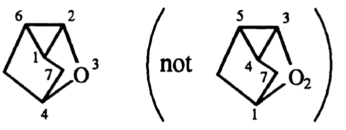
VB-8.1 Low locants are allocated for heteroatoms indicated by replacement terms considered together as a set in ascending numerical order.

Examples



3,6,8-trioxabicyclo[3.2.2]nonane

not 3,7,9-trioxabicyclo[3.2.2]nonane (3,**6**,8 is lower than 3,**7**,9)

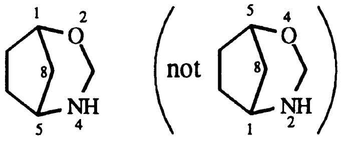


However 3-oxatricyclo[2.2.1.$0^{2,6}$]heptane

not 2-oxatricyclo[2.2.1.$0^{3,5}$]heptane (the bridge locants determine the numbering; 2,6 is lower than 3,5; see VB-6.4)

VB-8.1.1 Low locants are allocated for heteroatoms in the order of RB-1.4 [13], R-2.3.3 and R-9.3 [7].

Example

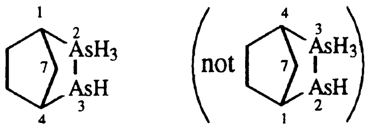


2-oxa-4-azabicyclo[3.2.1]octane

not 4-oxa-2-azabicyclo[3.2.1]octane (2-oxa is lower than 4-oxa)

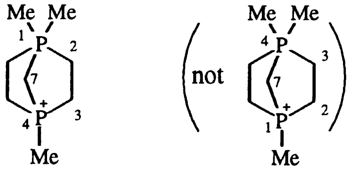
VB-8.1.2 Low locants are allocated for nonstandard valency expressed by the λ symbol [8], if necessary in order of decreasing numerical value of the bonding number, i.e. lower numbers for λ^6 rather than λ^4.

Examples



$2\lambda^5$,3-diarsabicyclo[2.2.1]heptane

not 2,$3\lambda^5$-diarsabicyclo[2.2.1]heptane (2 is lower than 3)

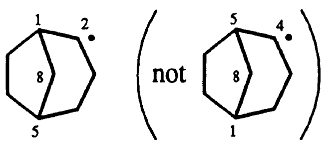


1,1,4-trimethyl-$1\lambda^5$,4-diphosphabicyclo[2.2.1]heptan-4-ium

not 1,4,4-trimethyl-1,$4\lambda^5$-diphosphabicyclo[2.2.1]heptan-1-ium ($1\lambda^5$ is lower than $4\lambda^5$)

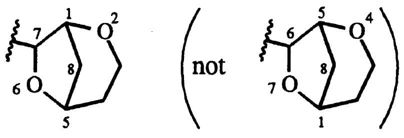
VB-8.1.3 Low locants are allocated for radical sites, or if the ring system is a substituent, its point of attachment.

Examples



bicyclo[3.2.1]octan-2-yl

not bicyclo[3.2.1]octan-4-yl (2 is lower than 4)



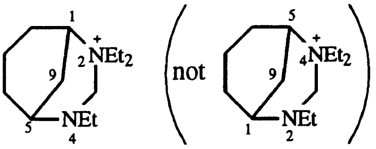
However 2,6-dioxabicyclo[3.2.1]octan-7-yl

not 4,7-dioxabicyclo[3.2.1]octan-6-yl (2,6 is lower than 4,7, see VB-8.1)

Note: In previous editions of these rules (A-31.4 and B-14.1, [6]) octan-yl was contracted to oct-yl [however, see R-2.5 and R-5.8.1 [7] and RC-81.1.2 [9] where the contraction is not used].

VB-8.1.4 Low locants are allocated for cationic sites.

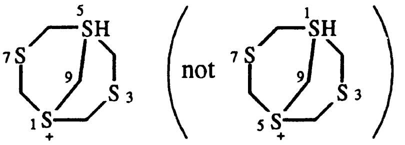
Examples



2,2,4-triethyl-2,4-diazabicyclo[3.3.1]nonan-2-ium (preferred name)

Alternative name 2,2,4-triethyl-4-aza-2-azoniabicyclo[3.3.1]nonane

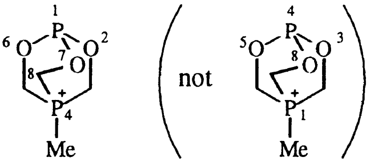
not 2,4,4-triethyl-2,4-diazabicyclo[3.3.1]nonan-4-ium (2-ium is lower than 4-ium)



1λ^4,3,5λ^4,7-tetrathiabicyclo[3.3.1]nonan-1-ylium (preferred name)

Alternative name 3,5λ^4,7-trithia-1-thioniabicyclo[3.3.1]nonane

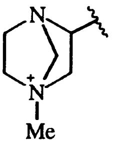
not 1λ^4,3,5λ^4,7-tetrathiabicyclo[3.3.1]nonan-5-ylium (1-ylium is lower than 5-ylium)



4-methyl-2,6,7-trioxa-1,4-diphosphabicyclo[2.2.2]octan-4-ium (preferred name)

Alternative name 4-methyl-2,6,7-trioxa-1-phospha-4-phosphoniabicyclo[2.2.2]octane

not 1-methyl-3,5,8-trioxa-1,4-diphosphabicyclo[2.2.2]octan-1-ium (1,2,4,6,7 is lower than 1,3,4,5,8; see VB-8.1)

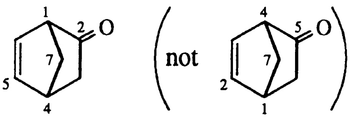


However 4-methyl-1,4-diazabicyclo[2.2.1]heptan-4-ium-2-yl

not 1-methyl-1,4-diazabicyclo[2.2.1]heptan-1-ium-3-yl (2 is lower than 3 for free valence; see VB-8.1.3)

VB-8.2 Low locants are allocated for the principal functional groups.

Examples

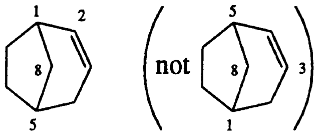


bicyclo[2.2.1]hept-5-en-2-one

not bicyclo[2.2.1]hept-2-en-5-one (2-one is lower than 5-one)

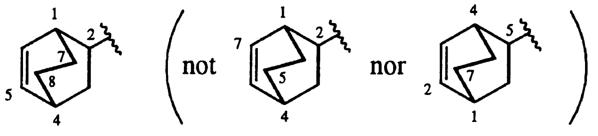
VB-8.3 Low locants are allocated for double bonds where the atoms of each double bond have consecutive locants. Only the lower of the two locants for each double bond is cited when they differ by one. If the two locants are not consecutive a compound locant is required, see VB-8.3.1. If a triple bond is present see VB-8.3.3.

Examples



bicyclo[3.2.1]oct-2-ene

not bicyclo[3.2.1]oct-3-ene (2 is lower than 3)



However bicyclo[2.2.2]oct-5-en-2-yl

not bicyclo[2.2.2]oct-7-en-2-yl (5 is lower than 7)

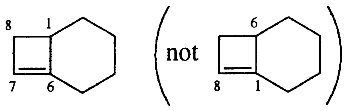
nor bicyclo[2.2.2]oct-2-en-5-yl (2 is lower than 5 for free valence, see VB-8.1.3)

If there is a choice of names or numbering the following criteria are considered in order until a decision is made.

VB-8.3.1 A minimum number of compound locants are selected. A compound locant is used for a double bond if the locants of the atoms at each end of the double bond do not differ by one. When a compound locant is required the higher locant is cited in parentheses. A benzene ring is named as a cyclohexatriene corresponding to the Kekulé structure with the preferred name. Other aromatic rings are treated similarly when necessary.

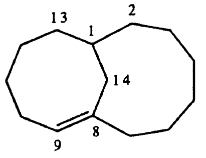
Note: This rule was used in the Nomenclature of Steroids [14] rule 3S-2.5(2), e.g. estra-5,7,9-triene is recommended rather than estra-5(10),6,8-triene.

Examples



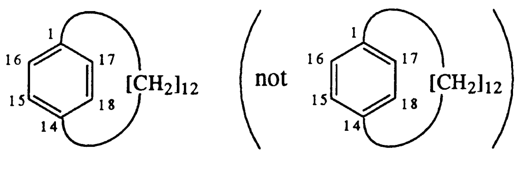
bicyclo[4.2.0]oct-6-ene (also CAS index name)

not bicyclo[4.2.0]oct-1(8)-ene (single locant rather than compound locant)



bicyclo[6.5.1]tetradec-8-ene

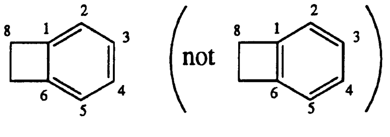
not bicyclo[6.5.1]tetradec-1(13)-ene (this is a change from R-3.1.1, 7)



bicyclo[12.2.2]octadeca-1(16),14,17-triene

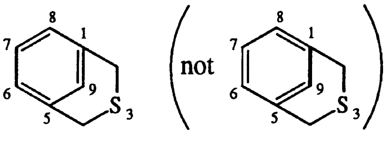
not bicyclo[12.2.2]octadeca-1(17),14(18),15-triene (1 compound locant rather than 2)

Note: This example from A-31.3 [6] is named there as bicyclo[12.2.2]octadeca-1(16),14,17-triene or bicyclo[12.2.2]octadeca-14,16(1),17-triene. The latter name, which is no longer recommended, corresponds to the CAS index name (bicyclo[12.2.2]octadeca-14,16,17-triene). CAS always orientates a ring system so that the main ring is numbered clockwise and thus the aromatic ring is numbered round the ring clockwise. A compound locant is not used by CAS when the second atom is obvious.



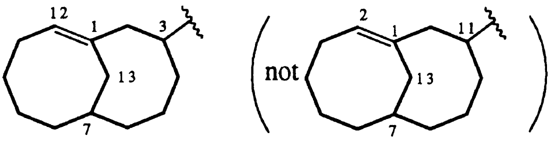
bicyclo[4.2.0]octa-1,3,5-triene (also CAS index name)

not bicyclo[4.2.0]octa-1(6),2,4-triene (all single locants selected)



3-thiabicyclo[3.3.1]nona-1(9),5,7-triene (also CAS index name)

not 3-thiabicyclo[3.3.1]nona-1(8),5(9),6-triene (1 compound locant rather than 2)

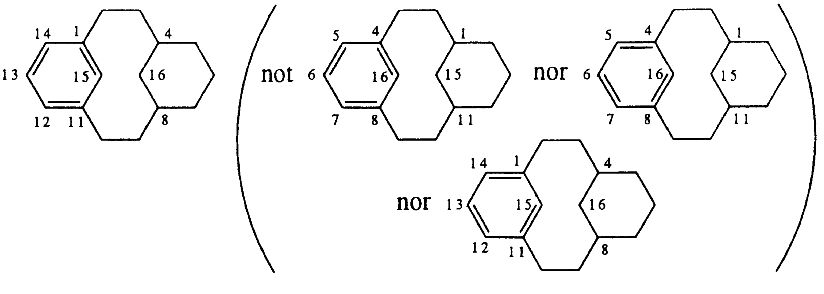


However bicyclo[5.5.1]tridec-1(12)-en-3-yl

not bicyclo[5.5.1]tridec-1-en-11-yl (3 is lower than 11, see VB-8.1.3)

VB-8.3.2 When comparing double bond locants including compound locants any numbers in parentheses are ignored.

Examples

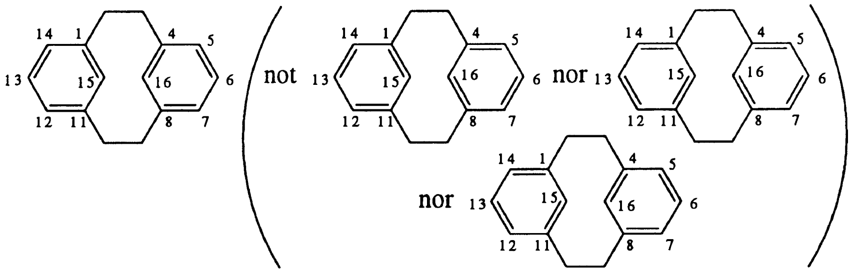


tricyclo[9.3.1.1^{4,8}]hexadeca-1(15),11,13-triene

not tricyclo[9.3.1.1^{4,8}]hexadeca-4(16),5,7-triene

nor tricyclo[9.3.1.1^{4,8}]hexadeca-4,6,8(16)-triene (1,11,13 is lower than 4,5,7 or 4,6,8)

nor tricyclo[9.3.1.1^{4,8}]hexadeca-1(14),11(15),12-triene (1 compound locant rather than 2, see VB-8.3.1)



tricyclo[9.3.1.$1^{4,8}$]hexadeca-1(15),4(16),5,7,11,13-hexaene

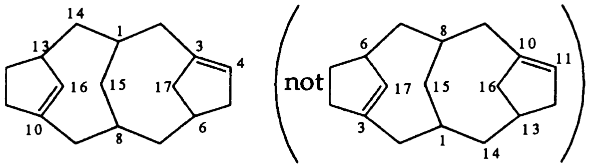
not tricyclo[9.3.1.$1^{4,8}$]hexadeca-1(15),4,6,8(16),11,13-hexaene (CAS index name) [1,4,**5**,7,11,13 is lower than 1,4,**6**,8,11,13]

nor tricyclo[9.3.1.$1^{4,8}$]hexadeca-1(14),4,6,8(16),11(15),12-hexaene (2 compound locants is lower than 3, see VB-8.3.1)

nor tricyclo[9.3.1.$1^{4,8}$]hexadeca-1(14),4(16),5,7,11(15),12-hexaene (2 compound locants is lower than 3, see VB-8.3.1)

If there is still a choice low locants are selected considering all locants as a set.

Example

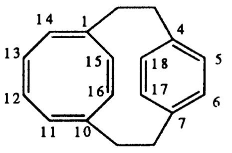


tetracyclo[6.6.1.$1^{3,6}$.$1^{10,13}$]heptadeca-3,10(16)-diene

not tetracyclo[6.6.1.$1^{3,6}$.$1^{10,13}$]heptadeca-3(17),10-diene (3,10,**16** is lower than 3,10,**17**)

Note: Under some circumstances (e.g. [15]) localised double bonds have been recognised in an apparently fully conjugated ring. The specific localisation of the double bonds can be indicated by the prefix Δ with a superscript locant (or compound locant) of the lowest numbered relevant double bond (see FR-9.2 [12]; footnote to B-1.2 [6]).

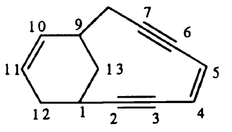
Example



$\Delta^{1(14)}$-tricyclo[8.4.2.$2^{4,7}$]octadeca-1(14),4,6,10,12,15,17-heptaene

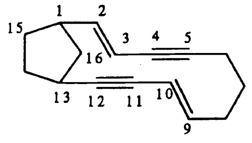
VB-8.3.3 If there are both double and triple bonds present lower locants are selected for multiple bonds as a set, then lower locants for the double bonds.

Examples



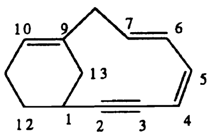
bicyclo[7.3.1]trideca-4,10-diene-2,6-diyne

not bicyclo[7.3.1]trideca-5,11-diene-3,7-diyne (**2**,4,6,10 is lower than **3**,5,7,11)



bicyclo[11.2.1]hexadeca-2,9-diene-4,11-diyne

not bicyclo[11.2.1]hexadeca-4,11-diene-2,9-diyne (both 2,4,9,11 but **2**,9 is lower than **4**,11)

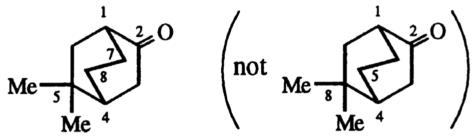


However bicyclo[7.2.1]trideca-4,6,9-trien-2-yne

not bicyclo[7.2.1]trideca-1(12),3,5-trien-7-yne (no compound locant, see VB-8.3.1)

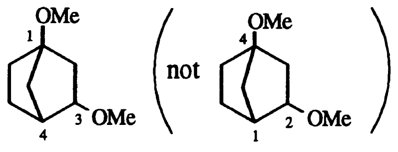
VB-8.4 Lower locants are allocated for substituents cited by prefixes.

Examples



5,5-dimethylbicyclo[2.2.2]octan-2-one

not 8,8-dimethylbicyclo[2.2.2]octan-2-one (5,5 is lower than 8,8)

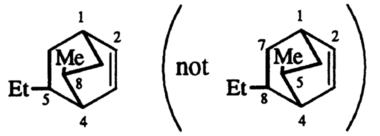


1,3-dimethoxybicyclo[2.2.1]heptane

not 2,4-dimethoxybicyclo[2.2.1]heptane (1,3 is lower than 2,4)

VB-8.4.1 Low locants are allocated for substituent prefixes in the order of their citation.

Example

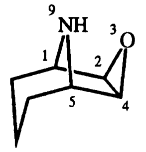


5-ethyl-8-methylbicyclo[2.2.2]oct-2-ene

not 8-ethyl-5-methylbicyclo[2.2.2]oct-2-ene (5-ethyl is lower than 8-ethyl)

VB-8.5 *R* is selected rather than *S* to indicate configuration.

Examples



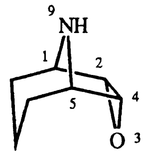
(1*R*,2*R*,4*S*,5*S*)-3-oxa-9-azatricyclo[3.3.1.0^{2,4}]nonane

not (1*S*,2*S*,4*R*,5*R*)-3-oxa-9-azatricyclo[3.3.1.0^{2,4}]nonane (1*R* rather than 1*S*)

Beilstein name = (1*rN*^{9},2*tH*,4*tH*)-3-oxa-9-azatricyclo[3.3.1.0^{2,4}]nonane

CAS index name = (1α,2β,4β,5α)-3-oxa-9-azatricyclo[3.3.1.0^{2,4}]nonane

Note: The above example could also be described as *exo*- by extrapolation of the term used to describe substituents on a bicyclic bridge compound. Similarly the example below would be *endo*-. However this system is not recommended as it would be difficult to extend it to tetracyclic systems and even tricyclic systems where it is difficult to identify the bicyclic system used to identify *exo/endo*.



(1*R*,2*S*,4*R*,5*S*)-3-oxa-9-azatricyclo[3.3.1.0^{2,4}]nonane

not (1*S*,2*R*,4*S*,5*R*)-3-oxa-9-azatricyclo[3.3.1.0^{2,4}]nonane (1*R* rather than 1*S*)

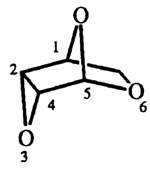
Beilstein name = (1*rN*^{9},2*cH*,4*cH*)-3-oxa-9-azatricyclo[3.3.1.0^{2,4}]nonane

CAS index name = (1α,2α,4α,5α)-3-oxa-9-azatricyclo[3.3.1.0^{2,4}]nonane

VB-9 Configuration of chiral systems

The configuration of a chiral ring system with a unique numbering determined by the structure is specified by the *R/S* system. It may thus be necessary to specify whether the name refers to one enantiomer, a racemate, or is only indicating relative configuration.

Example



(1*S*,2*R*,4*R*,5*S*)-3,6,8-trioxatricyclo[3.2.1.0^{2,4}]octane

CAS index name = [1*S*-(1α,2α,4α,5α)]-3,6,8-trioxatricyclo[3.2.1.0^{2,4}]octane

Note: A different method of indicating stereochemistry has been adopted by CAS starting with volume **129** of *Chemical Abstracts*. This would also apply to the names given in VB-8.5.

If it is required to specify that this name applies to a racemate, or that only the relative stereochemistry is known the prefixes *rac*- or *rel*- may be used. Thus for the example above:

This example	(1*S*,2*R*,4*R*,5*S*)-3,6,8-trioxatricyclo[3.2.1.$0^{2,4}$]octane
Its enantiomer	(1*R*,2*S*,4*S*,5*R*)-3,6,8-trioxatricyclo[3.2.1.$0^{2,4}$]octane
Racemic sample	(1*RS*,2*SR*,4*SR*,5*RS*)-3,6,8-trioxatricyclo[3.2.1.$0^{2,4}$]octane
or	*rac*-(1*R*,2*S*,4*S*,5*R*)-3,6,8-trioxatricyclo[3.2.1.$0^{2,4}$]octane
Relative configuration only	(1*R**,2*S**,4*S**,5*R**)-3,6,8-trioxatricyclo[3.2.1.$0^{2,4}$]octane
or	*rel*-(1*R*,2*S*,4*S*,5*R*)-3,6,8-trioxatricyclo[3.2.1.$0^{2,4}$]octane

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