

# INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

ORGANIC CHEMISTRY DIVISION  
COMMISSION ON NOMENCLATURE OF ORGANIC CHEMISTRY\*

## NOMENCLATURE FOR CYCLIC ORGANIC COMPOUNDS WITH CONTIGUOUS FORMAL DOUBLE BONDS (THE $\delta$ -CONVENTION)

(Recommendations 1988)

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# Nomenclature for cyclic organic compounds with contiguous formal double bonds (the $\delta$ -convention) (Recommendations 1988)

Substitutive (organic) nomenclature requires that the number of hydrogen atoms, if any, on each skeletal atom of a parent be known unambiguously. Trivial or semisystematic names are used to denote many rings and ring systems containing the maximum number of noncumulative double bonds. In order to use substitutive nomenclature and the same skeletal names when formal cumulative double bonds, actual or theoretical, are present in these rings and ring systems, a method for indicating the location of a cumulative double bond system is required. Techniques used up to now are either cumbersome or tend to use established techniques in ways other than for which they were designed. The  $\lambda$ -convention (ref. 1) for specifying nonstandard valency states of skeletal atoms, although useful, is not by itself sufficient for this purpose.

These rules provide a method for unambiguously denoting the presence of cumulative double bonds at a skeletal atom in a ring or ring system that otherwise has the maximum number of noncumulative double bonds. When combined with the  $\lambda$ -convention, where necessary, the number of hydrogen atoms available for substitution on such skeletal atoms is unambiguously known. The basic principles of this method were introduced briefly in Section D of the IUPAC Organic Rules as revised for publication in the 1979 edition (ref. 2).

The  $\delta$ -convention is fully consistent with the fundamental principles of substitutive nomenclature, which are based on formalized bonding in structural diagrams, and are applicable to organic derivatives of inorganic rings and ring systems. It consists of a symbol,  $\delta^c$ , where c is an arabic number representing the number of double bonds attached to the skeletal atom indicated by the preceding locant. A nonstandard valence state of the skeletal atom is given by the  $\lambda$ -convention, where necessary.

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## INTRODUCTION

The presence of contiguous double bonds in chains and rings named as saturated systems is conveniently indicated by subtractive suffixes such as "-diene", "-triene", etc. (ref. 2a); for example, hexa-2,3-diene (2,3-hexadiene)\*, cycloocta-1,2,3-triene (1,2,3-cyclooctatriene)\*, 4-azabicyclo[8.2.2]tetradeca-2,3-diene, spiro[4.10]pentadeca-7,8,9-triene.

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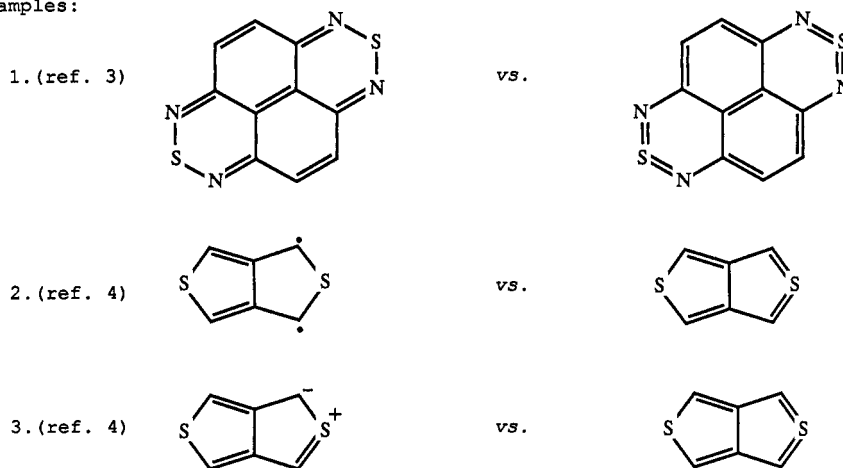
\*In the next edition of the IUPAC Organic Rules, locants will be placed within a name just ahead of the syllable to which they refer; however, it will not be wrong to place the locants elsewhere, such as in front of the name or after the name, as in French, provided that there is no ambiguity.

However, nomenclature for many rings and ring systems depends on the concept of the maximum number of noncumulative double bonds (ref. 2b); many trivial names for rings and ring systems and the system of fusion nomenclature rely on this principle for an accurate interpretation of the parent ring structure. The presence of contiguous double bonds in such systems (whether known structures or theoretical ones) has long been a serious problem in nomenclature, the difficulty being essentially that of defining clearly which skeletal atoms have hydrogen atoms attached.

Although the representation of a structure using contiguous double bonds is merely a formalism, it is especially convenient for nomenclature purposes. Names for such structures discussed in this report are not intended to carry implications of any kind as to the nature of the bonding actually present in the molecule. Similarly, the structures shown in this report indicate only the location of double bonds; no attempt is made to represent actual stereochemistry, such as in a linear cumulene carbon system.

It is generally useful, and often essential, especially for theoretical discussions, to have a name which unambiguously specifies the exact formal structure under discussion.

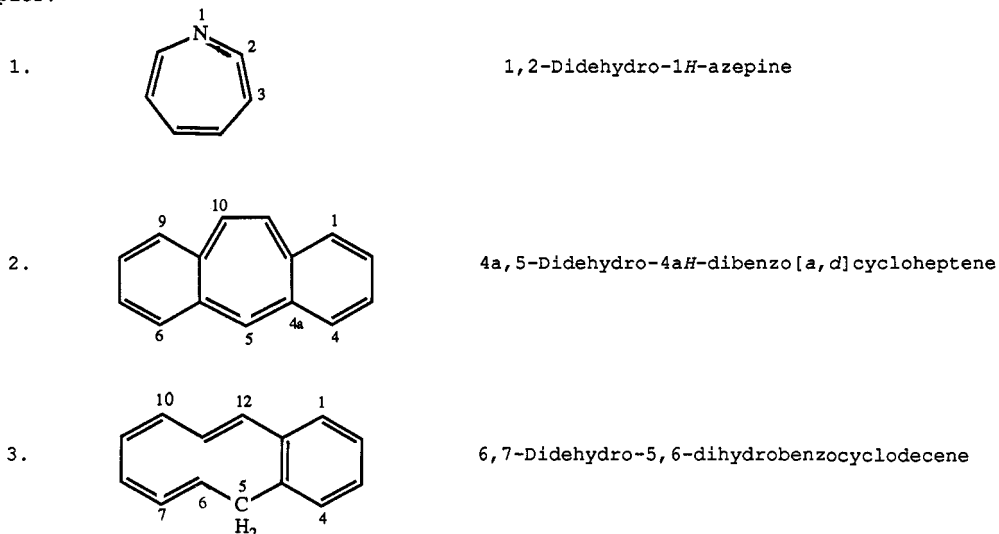
Examples:

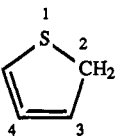


Theory and nomenclature are thus closely related and nomenclature has the difficult task of striking a balance between the wealth of theoretical knowledge about chemical structures and the necessity of devising relatively simple methods to be used by a variety of chemists, including many with little interest in theoretical aspects of chemical bonding.

The dehydro prefix, sometimes combined with the hydro prefix, can be used to indicate contiguous double bonds in rings and ring systems, whose names normally imply the maximum number of noncumulative double bonds.

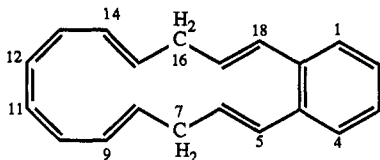
Examples:



4.  3,4-Didehydro-2,3-dihydrothiophene  
(this compound has also been called 2*H*-thiophene; however, the use of indicated hydrogen in this name is not consistent with the description of its use in Rule A-21.6 (ref. 2c))

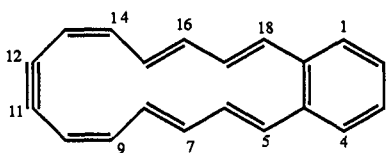
This technique can be quite cumbersome particularly when used in combination with "hydro" prefixes. It also allows different ways of drawing multiple bonds in some ring systems.

Example:

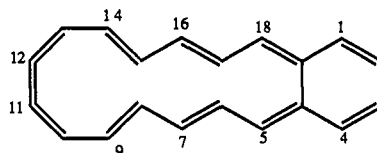


11,12-Didehydro-7,16-dihydrobenzocyclohexadecene

compare with:



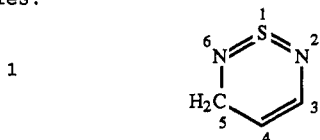
and



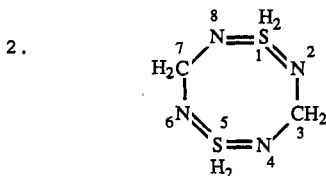
both of which can be named: 11,12-Didehydrobenzocyclohexadecene

Even more complications can occur when heteroatoms in nonstandard valence states are involved; techniques involving only the designation of the nonstandard valence states of the heteroatoms have usually been used, where needed, and the results are sometimes ambiguous.

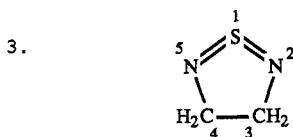
Examples:



1,1,2,6-Tetrahydro-1,1,5,6-tetrahydro-2*H*-1,2,6-thiadiazine (also known as 3*H*-1,2,6-Thia(*S*<sup>IV</sup>) diazine)



1,1,2,4,5,5,6,8-Octahydro-1,1,1,1,5,5,5,8-dithiatetrazocane (also known as 1*H*,1*H*,3*H*,5*H*,5*H*,7*H*-1,5,2,4,6,8-Dithia(1,5-*S*<sup>VI</sup>)tetrazocine; however, use of indicated hydrogen in this name is not consistent with the description of its use in Rule A-21.6 (ref. 2c))



1,1,2,5-Tetrahydro-1,2,3,4,5-hexahydro-1,2,5-thiadiazole  
1,1,2,5-Tetrahydro-1,1-dihydro-1,2,5-thiadiazolidine (also known as 3,4-dihydro-1,2,5-thia(*S*<sup>IV</sup>) diazole)

The  $\lambda$ -convention (ref. 1) has solved problems of designating nonstandard valence states of skeletal atoms including even carbon atoms. This includes rings and ring systems with the maximum number of noncumulative double bonds; however, it alone is not always sufficient to describe systems with cumulative double bonds unambiguously. Therefore, the symbol  $\delta^c$ , where  $c$  is the number of skeletal double bonds terminating at a skeletal heteroatom was introduced into Section D of the IUPAC Organic Rules as revised for the 1979 edition (ref. 2d).

This report now describes the details of the  $\delta$ -convention, and its applicability to cyclic hydrocarbons as well as to heterocycles. Although skeletal atoms of "normal" cyclic parent hydrides, i.e., those having only the maximum number of noncumulative double bonds, could be described by  $\delta^c$ , where  $c = 1$ , there is no reason to do so just as there is no reason to cite a  $\lambda^n$  symbol for a skeletal atom in its "standard" valence state. Furthermore, although a saturated skeletal atom could be indicated by  $\delta^c$ , where  $c = 0$ , there is no reason to replace

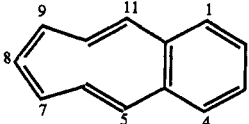
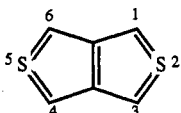
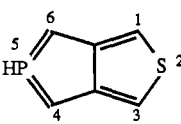
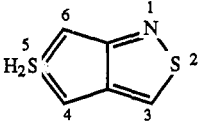
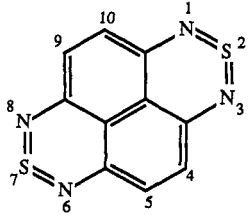
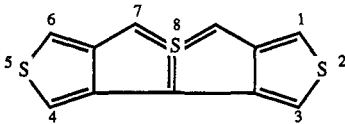
the technique of indicated hydrogen at this time.

The technique described in this report for designating contiguous double bonds in cyclic parent hydrides could be extended to the designation of triple bonds by using a symbol such as  $\tau^c$ . Here, however, the use of the symbolism when  $c = 1$  would be necessary. In addition, a combination of the symbols  $\delta$  and  $\tau$  could be used to describe a skeletal atom to which both a double bond and a triple bond are attached, i. e.,  $\delta^1 \tau^1$ .

## RECOMMENDATIONS

**De-1. The  $\delta^c$ -symbol** In describing the presence of contiguous double bonds in a cyclic parent hydride whose name normally implies the maximum number of noncumulative double bonds, a skeletal atom at which more than one double bond terminates is qualified by the symbol  $\delta^c$ , where  $c$  is an arabic number representing the number of double bonds. The  $\delta^c$  symbol is cited immediately after an expressed locant for the skeletal atom in the name of the parent hydride and follows the  $\lambda^n$  symbol, if present. If the locant for the skeletal atom is not expressed in the name, the locant, if necessary, and the  $\delta^c$  symbol are cited in front of the name of the parent hydride, but after any required indicated hydrogen (see De-2).

Examples:\*

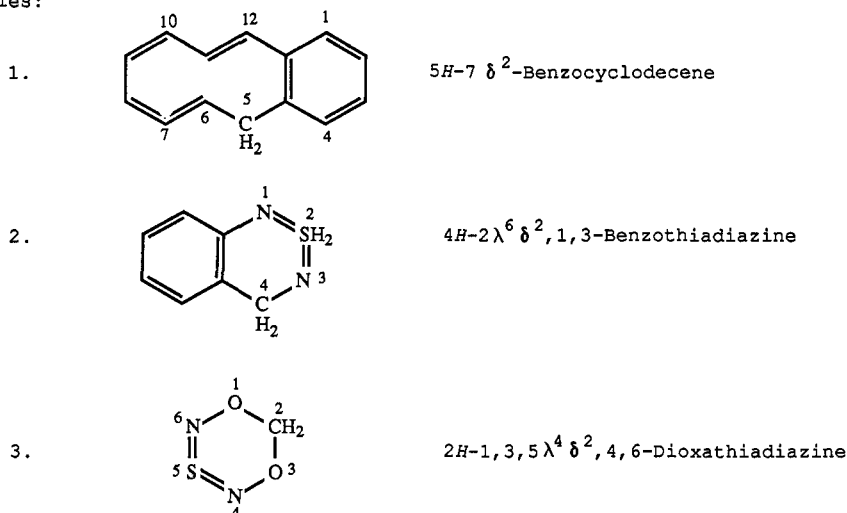
1.   $8 \delta^2$ -Benzocyclonene
2.   $2 \lambda^4 \delta^2, 5 \lambda^4 \delta^2$ -Thieno[3,4-c]thiophene
3.   $5 \lambda^5 \delta^2$ -Phospholo[3,4-c]thiophene
4.   $5 \lambda^6 \delta^2$ -Thieno[3,4-c]isothiazole
5.   $2 \lambda^4 \delta^2, 7 \lambda^4 \delta^2$ -Naphtho[1,8-cd:4,5-c'd']-bis[1,2,6]thiadiazine
6.   $8 \lambda^6 \delta^3$ -Thieno[3,4-c]thieno[3',4':3,4]=thieno[1,2-a]thiophene  
 $2,5,7a \lambda^6 \delta^3$ -Trithiadicyclopenta[a,f]pentalene

\*Examples 2, 3, 4, and 6 may be represented by other contributing structures which are named in an analogous way; for example, compare example 2 with example 3 under De-3.

**De-2. Indicated hydrogen** After contiguous double bonds have been inserted into a parent ring structure and the maximum number of noncumulative double bonds has been assigned to the remaining parent structure, taking account of the modified valence of any ring atom with a nonstandard bonding number, any ring atom with a bonding number of three or higher, and carrying one or more hydrogen atoms, is designated by the "indicated hydrogen" symbolism as described in Rule A-21.6 (ref. 2c).

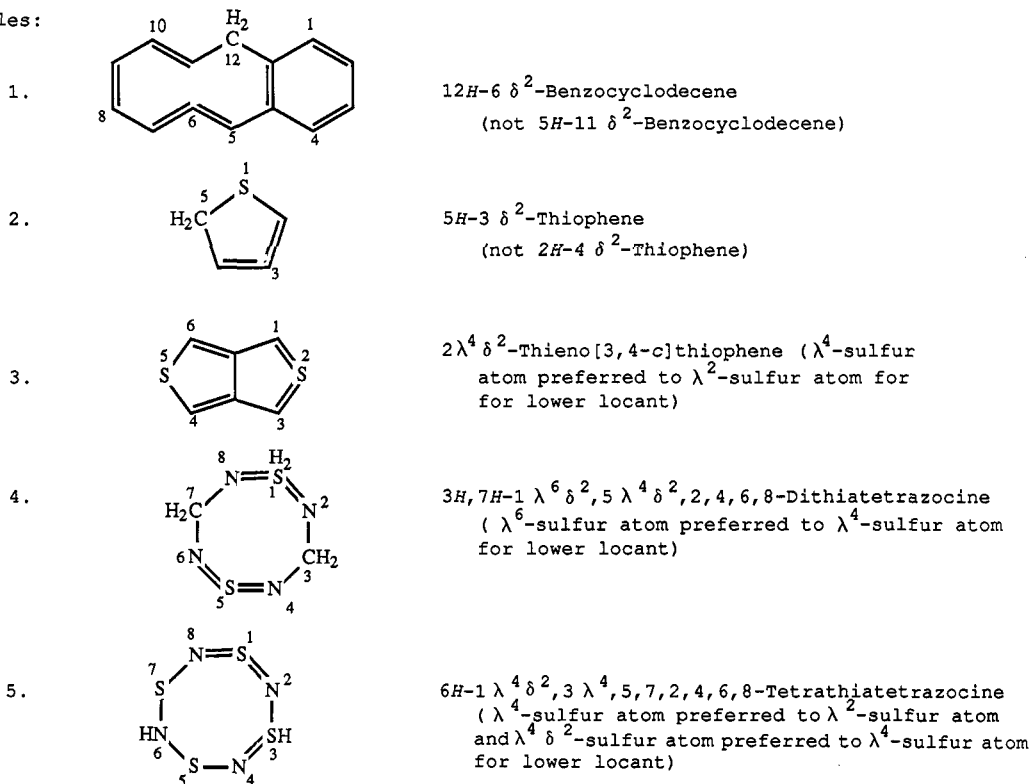
**Note.** Designation of indicated hydrogen at nonbridgehead ring positions between two bivalent ring atoms is often omitted.

Examples:



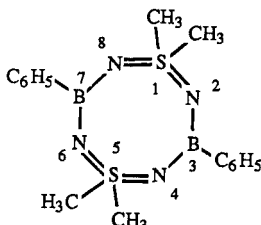
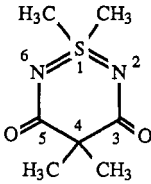
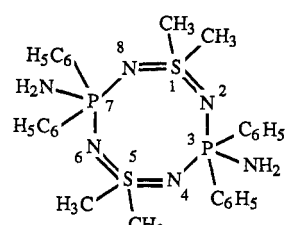
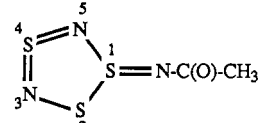
**De-3. Numbering** When there is a choice for numbering in a cyclic parent hydride after the heteroatoms have been numbered according to the principles of Section B (ref. 2e) followed by preferences for nonstandard valence states in order of decreasing bonding number value (ref. 1a) (see examples 3 and 4, below), preference then is given to skeletal atoms in decreasing order of number of double bonds terminating at the skeletal atom and then to indicated hydrogen positions.

Examples:

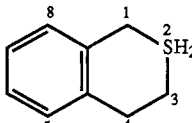


**De-4. Derivatives** of cyclic parent hydrides with contiguous double bonds formally derived by substitution of hydrogen atoms are named by using prefixes and/or suffixes in the established manner (ref. 2). Prefixes for describing substituents derived from these cyclic parent hydrides are formed in the usual way by using endings such as "-yl", "-ylidene", "-diyl", etc. (ref. 2).

Examples:

1.  1,1,5,5-Tetramethyl-3,7-diphenyl-3H,7H- $1\lambda^6\delta^2,5\lambda^6\delta^2$ -2,4,6,8,3,7-dithiatetraza-diborocine
2.  1,1,4,4-Tetramethyl-3H- $1\lambda^6\delta^2,2,6$ -thiadiazine-3,5(4H)-dione
3.  1,1,5,5-Tetramethyl-3,3,7,7-tetraphenyl-3H,7H- $1\lambda^6\delta^2,5\lambda^6\delta^2,2,4,6,8,3\lambda^5,7\lambda^5$ -dithia-tetrazadiphosphocine-3,7-diamine
4.  N-(1H- $1\lambda^4,2,4\lambda^4\delta^2,3,5$ -Trithiadiazol-1-ylidene)acetamide

**Note:** If a saturated ring atom is to be generated by hydro prefixes the parent ring should not denote the presence of contiguous double terminating at the skeletal atom.

- Example:  1,2,3,4-Tetrahydro-2 $\lambda^4$ -benzothiopyran (not 1,2,2,3-Tetrahydro-4H-2 $\lambda^4\delta^2$ -benzothiopyran)

## REFERENCES

1. International Union of Pure and Applied Chemistry. Organic Chemistry Division. Commission on Nomenclature of Organic Chemistry, "Treatment of Variable Valence in Organic Nomenclature (Lambda Convention), Recommendations 1983", *Pure Appl. Chem.* **56**, 769-778 (1984); (a) Rule Lm-2.0.
2. International Union of Pure and Applied Chemistry. Organic Chemistry Division. Commission on Nomenclature of Organic Chemistry, "Nomenclature of Organic Chemistry", Sections A, B, C, D, E, F, and H, Pergamon Press, Oxford, 1979; (a) Rules A-3, pp. 11-14; A-11.3, p. 16; A-31.3, p. 32; and A-41.3, p. 38; (b) Rules A-21, pp. 20-25; B-1, B-2, and B-3, pp. 53-68; (c) Rule A-21.6, p. 25; (d) Subsection D-0.3 Terminology; Bonding number, p. 325; (e) Section B, pp. 53-76.
3. J. P. Boutique, J. Riga, J. J. Verbist, J. Delhalle, J. G. Firpiat, J. M. Andre, R. C. Haddon, and M. L. Kaplan, *J. Am. Chem. Soc.* **104**, 2691-2697 (1982).
4. M. P. Cava and M. V. Lakshmikantham, *Acc. Chem. Res.* **8**, 139-144 (1975).