

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

1957 REPORT OF THE COMMISSION ON THE NOMENCLATURE OF ORGANIC CHEMISTRY

Definitive Rules for Nomenclature of Organic Chemistry

These Rules shall be known as the IUPAC 1957 Rules.

Section A. Hydrocarbons

Section B. Fundamental Heterocyclic Systems

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INTRODUCTION

The first international proposals on the nomenclature of organic chemistry, made at Geneva in 1892, were revised and extended by the Definitive Report of the Commission for the Reform of Nomenclature in Organic Chemistry of the International Union of Chemistry (I.U.C.) which appeared after the meeting at Liège in 1930 (Liège Rules), and was supplemented by less extensive reports from the meetings at Lucerne in 1936 and at Rome in 1938. Although these proposals rendered great service, it was apparent at the meeting of the International Union of Pure and Applied Chemistry at London in 1947 that, in some matters, extension and revision of the nomenclature rules for organic chemistry were required. Those who have served on the Commission on Nomenclature of Organic Chemistry for varying periods from 1947 to date (1957) are: M. Betti,* R. S. Cahn, L. T. Capell, G. Dupont, G. M. Dyson, C. S. Gibson,* G. Kersaint, N. Lozac'h, R. Marquis,* A. D. Mitchell, H. S. Nutting, A. M. Patterson,* V. Prelog, F. Richter, S. Veibel, P. E. Verkade and E. Votocek.*

The Commission's progress in the period 1947 to 1955, inclusive, has been reported in successive issues of the *Comptes Rendus* of the Conferences of the Union. Relevant parts of those reports are included, with a few revisions, in the rules which form the body of this publication.

* Deceased.

General Principles

The Commission believes that differences in nomenclature frequently hinder the accurate and intelligible conveyance of information from one chemist to another, so tending to hamper understanding and progress. The Commission urges conformity with internationally agreed nomenclature even when this nomenclature may not seem the best possible from the point of view of the chemists of a particular nation or group.

The rules now presented are intended to be suitable for textbooks, journals and patents, for lexicons and similar compilations, and for indexes, even if not always wholly so for conversation or lectures. The rules will be issued in parts, as they become approved by the Union. They constitute recommendations for the naming of types of compounds and of individual compounds. They are not exhaustive, except in specified cases. Where, for various reasons, limitation to a single method of nomenclature appears undesirable or impossible, alternatives are given; but the Commission hopes that elimination of alternatives may become acceptable as the merits of one method become more generally recognized. The Commission hopes also that each nation will try to reduce the variations in nomenclature with regard to spelling, the position of numbers, punctuation, italicizing, abbreviations, elision of vowels, certain terminations, and so forth; the present rules are not to be held as making recommendations in these matters; the rules are written in accord with the conventions of *Chemical Abstracts* (except where specifically stated otherwise), but solely for uniformity from one rule to another.

Owing to the very extensive nomenclature which has come into being since the last revision, the Commission has, in the main, confined its efforts to codifying sound practices which already existed, rather than to originating new nomenclature—the latter may form a later stage of the Commission's activities.

In so doing, the Commission had in mind the following main principles: (a) as few changes as

possible should be made in existing nomenclature, though utility is more important than priority; (b) rules and names should be unequivocal and unique, but simple and concise; (c) records in journals, abstracts, compendia, and industry should be used to assess the relative extent of past use of various alternatives; (d) rules should be consistent with one another, yet aid expression in the particular field of chemistry involved and be capable of extension with the progress of science; (e) trivial names, and names having only a very small systematic component, cannot be eliminated when in very common use, but those of less value should be replaced by systematic (or at least more systematic) ones, and the creation of new trivial names should be discouraged by provision of extensible systematic nomenclature; (f) names should be adaptable to different languages. The Commission is aware that acceptance of its recommendations depends in large measure on the success which has attended its attempts to assess, for each particular case, the relative merits of these often conflicting claims.

Glossary

The Commission considered it unnecessary to define chemical terms in common use. However, certain terms which have special meaning in nomenclature merit brief description, namely:

Parent name: that part of the name from which a particular name is derived by a prescribed variation, *e.g.*, ethane giving rise to ethanol. Names often have more than one parent, *e.g.*, (chloromethyl)cyclohexane has methylcyclohexane as parent, which in turn has cyclohexane as its parent.

Systematic name: a name composed wholly of specially coined or selected syllables, with or without numerical prefixes, *e.g.*, pentane, oxazole.

Trivial name: a name no part of which is used in a systematic sense, *e.g.*, xanthophyll.

Semi-systematic name or semi-trivial name: a name of which only a part is used in a systematic sense, *e.g.*, methane (-ane), butene (-ene), calciferol (-ol). (Most names in organic chemistry belong to this class.)

Substitutive name: a name involving replacement of hydrogen by a group or by another element, *e.g.*, 1-methylnaphthalene, 1-pentanol.

Replacement name: an "a" name, where C, CH, or CH₂ is replaced by a hetero atom, *e.g.*, 2,7,9-triazaphenanthrene. Also, certain names involving thio- (also seleno- or telluro-) to indicate replacement of oxygen by sulfur (or selenium or tellurium, respectively), *e.g.*, thiopyran.

Subtractive name: a name involving removal of specified atoms, *e.g.*, in the aliphatic series names ending in -ene or -yne. Also names involving anhydro-, dehydro-, deoxy-, *etc.*, or nor-.

Radicalfunctional name: a name formed from the name of a radical and the name of a functional class, *e.g.*, acetyl chloride, ethyl alcohol.

Additive name: a name signifying addition between molecules and/or atoms, *e.g.*, styrene oxide.

Conjunctive name: a name formed by placing together the names of two molecules, it being understood that the two molecules are linked by loss of one hydrogen atom from each, *e.g.*, naphthalene-acetic acid.

Fusion name: a name for a cyclic system formed by use of a linking "o" between the names of two ring systems, denoting that the two systems are fused by two or more common atoms, *e.g.*, benzofuran.

Hantzsch-Widman name: a name for a heterocyclic system, as devised by Hantzsch and Widman, from a prefix or prefixes (to denote a hetero atom or atoms) and a suffix -ole or -ine (to denote a five- or a six-membered ring, respectively), *e.g.*, triazole, thiazole.

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Introductory Statement Concerning the Comments

Chemical Abstracts endeavors to follow the Rules of the International Union of Pure and Applied Chemistry in so far as is feasible for recording purposes, such as in the indexes. Exceptions are not numerous. It seems best to point out differences when such occur and to indicate a preference when alternate rules are given. This has been done by means of comments on individual rules. These comments are in smaller type, preceded by the symbol ♦.

RULES

A. HYDROCARBONS

Acyclic Hydrocarbons

A-1

1.1.—The first four saturated unbranched acyclic hydrocarbons are called methane, ethane, propane and butane. Names of the higher members of this series consist of a numerical prefix and the ter-

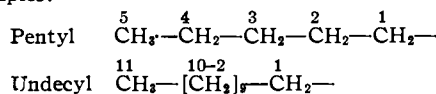
mination "-ane." Examples of these numerical prefixes are shown in the table below. The generic name of saturated acyclic hydrocarbons (branched or unbranched) is "alkane."

Examples: (*n* = total number of carbon atoms)

1	Methane	22	Docosane
2	Ethane	23	Tricosane
3	Propane	24	Tetracosane
4	Butane	25	Pentacosane
5	Pentane	26	Hexacosane
6	Hexane	27	Heptacosane
7	Heptane	28	Octacosane
8	Octane	29	Nonacosane
9	Nonane	30	Triacontane
10	Decane	31	Hentriacontane
11	Undecane	32	Dotriacontane
12	Dodecane	33	Trtriacontane
13	Tridecane	40	Tetracontane
14	Tetradecane	50	Pentacontane
15	Pentadecane	60	Hexacontane
16	Hexadecane	70	Heptacontane
17	Heptadecane	80	Octacontane
18	Octadecane	90	Nonacontane
19	Nonadecane	100	Hectane
20	Eicosane	132	Dotriacontahectane
21	Heneicosane		

1.2.—Univalent radicals derived from saturated unbranched acyclic hydrocarbons by removal of hydrogen from a terminal carbon atom are named by replacing the ending "-ane" of the name of the hydrocarbon by "-yl." The carbon atom with the free valence is numbered as 1. As a class, these radicals are called normal, or unbranched-chain, alkyls.

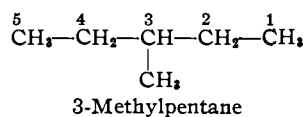
Examples:



A-2

2.1.—A saturated branched acyclic hydrocarbon is named by prefixing the designations of the side chains to the name of the longest chain present in the formula.

Example:



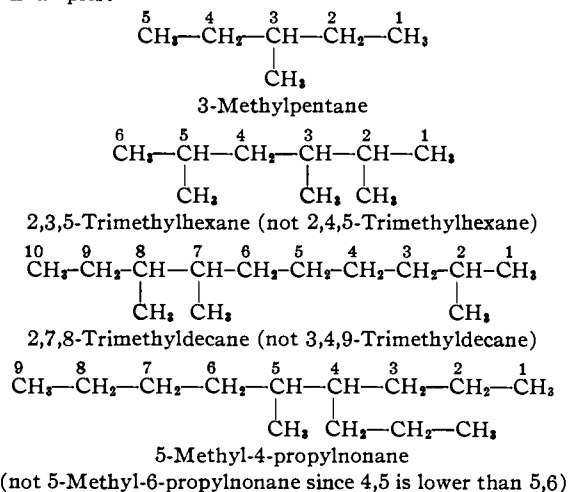
These names are retained for unsubstituted hydrocarbons only

Isobutane	(CH ₃) ₂ CH—CH ₃
Isopentane	(CH ₃) ₂ CH—CH ₂ —CH ₃
Neopentane	(CH ₃) ₄ C
Isohexane	(CH ₃) ₂ CH—CH ₂ —CH ₂ —CH ₃

◆ *Chemical Abstracts* index names for the above compounds are 2-methylpropane, 2-methylbutane, 2,2-dimethylpropane, and 2-methylpentane.

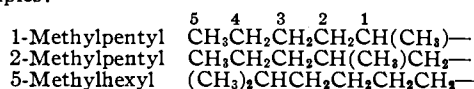
2.2.—The longest chain is numbered from one end to the other by arabic numerals, the direction being so chosen as to give the lowest numbers possible to the side chains. When series of locants containing the same number of terms are compared term by term, that series is "lowest" which contains the lowest number on the occasion of the first difference. This principle is applied irrespective of the nature of the substituents.

Examples:



2.25.—Univalent branched radicals derived from alkanes are named by prefixing the designation of the side chains to the name of the unbranched alkyl radical possessing the longest possible chain starting from the carbon atom with the free valence, the starting atom being numbered as 1.

Examples:



These names are retained for the unsubstituted radicals only

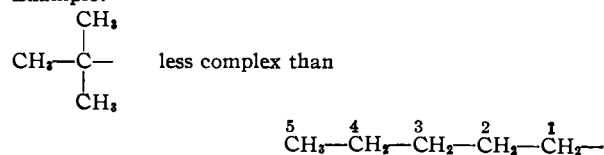
Isopropyl	(CH ₃) ₂ CH—
Isobutyl	(CH ₃) ₂ CHCH ₂ —
sec-Butyl	CH ₃ CH ₂ CH—
	CH ₃
tert-Butyl	(CH ₃) ₃ C—
Isopentyl	(CH ₃) ₂ CHCH ₂ CH ₂ —
Neopentyl	(CH ₃) ₃ CCH ₂ —
	CH ₃
tert-Pentyl	CH ₃ CH ₂ CH—
	CH ₃
Isohexyl	(CH ₃) ₂ CHCH ₂ CH ₂ CH ₂ —

2.3.—If two or more side chains of different nature are present, they may be cited (a) in order of increasing complexity or (b) in alphabetical order.

(a) The side chains are arranged in order of increasing complexity by applying the following criteria in series until a decision is reached:

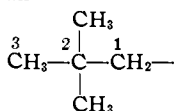
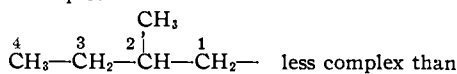
(i) The less complex is that containing the smaller total number of carbon atoms.

Example:

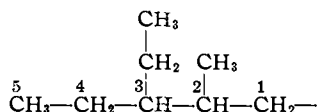
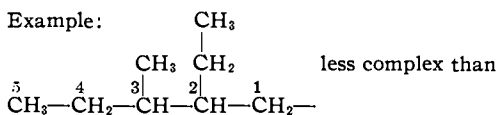


(ii) The less complex is that containing the longer straight chain.

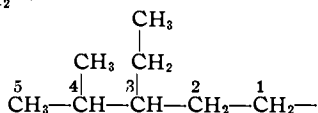
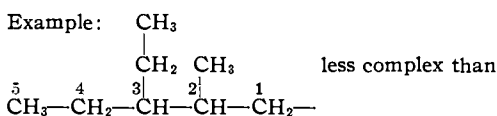
Example:



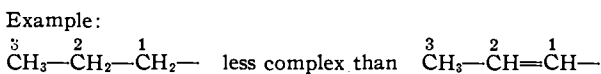
(iii) The less complex is that whose longest substituent has the lower locant.



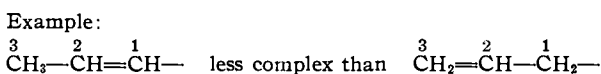
(iv) The less complex is that whose next longest substituent has the lower locant.



(v) The less complex is that which is the more saturated.

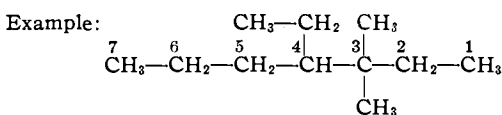


(vi) The less complex is that whose multiple linkage has the lower locant.



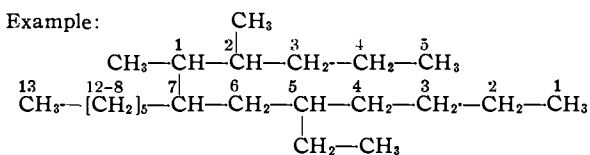
(b) The alphabetical order is decided as follows:

(i) The names of simple radicals are first alphabetized and the multiplying prefixes are then inserted.



ethyl is cited before methyl, thus 4-Ethyl-3,3-dimethylheptane

(ii) The name of a complex radical is considered to begin with the first letter of its complete name.

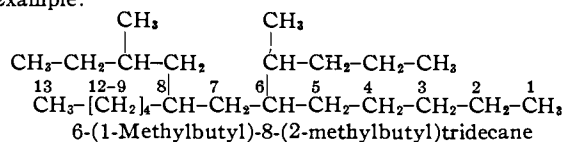


dimethylpentyl (as a complete single substituent) is alphabetized under "d," thus 7-(1,2-Dimethylpentyl)-5-ethyltridecane

(iii) In cases where complex radicals are composed of identical words, priority for citation is given to that radical which contains the lowest

locant at the first cited point of difference in the radical.

Example:

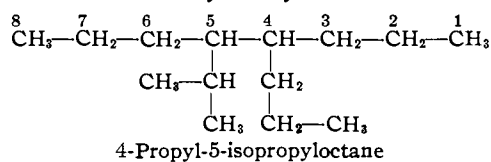
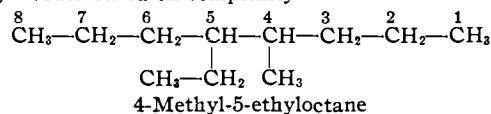


◆ *Chemical Abstracts* has long been a proponent of the alphabetical order for prefixes. The alphabetical order as given in A-2.3(b) is the order used by *Chemical Abstracts*.

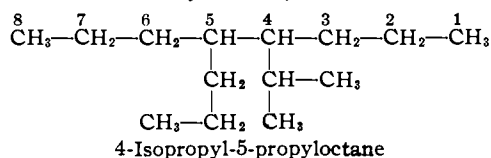
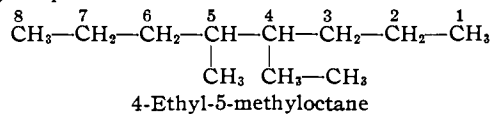
2.4.—If two or more side chains are in equivalent positions, the one to be assigned the lower number is that cited first in the name, whether the order of citation is based on complexity or on the alphabetical order.

Examples:

(a) Order based on complexity

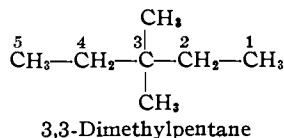


(b) Alphabetical order



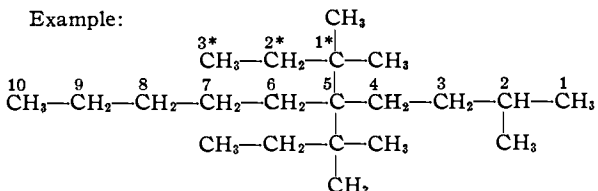
2.5.—The presence of identical unsubstituted radicals is indicated by the appropriate multiplying prefix di-, tri-, tetra-, penta-, hexa-, hepta-, octa-, nona-, deca-, undeca-, etc.

Examples:



The presence of identical radicals each substituted in the same way may be indicated by the appropriate multiplying prefix bis-, tris-, tetrakis-, pentakis-, etc. The complete expression denoting a side chain may be enclosed in parentheses or the carbon atoms in side chains may be indicated by primed numbers.

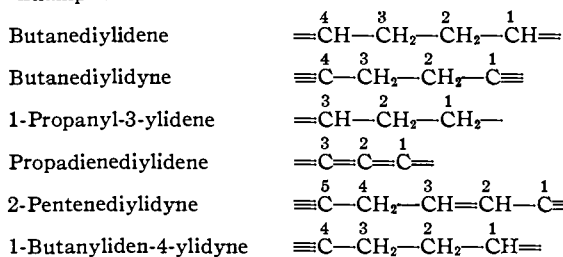
Example:



(a) Use of primes and order of complexity, * indicates primed numbers: 2-Methyl-5,5-bis-1',1'-dimethylpropyldecane.

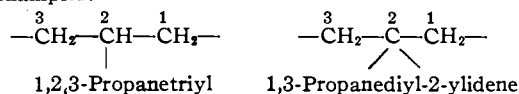
numbered in the order of "-yl," "-ylidene," "-ylidyne."

Examples:



4.5.—Multivalent radicals containing three or more carbon atoms with free valences at each end of a chain and additional free valences at intermediate carbon atoms are named by adding the endings "-triyl," "-tetrayl," "-diylidene," "diylidene," *etc.*, to the hydrocarbon name.

Examples:

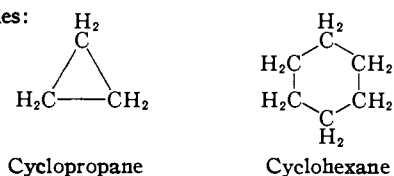


Monocyclic Hydrocarbons

A-11

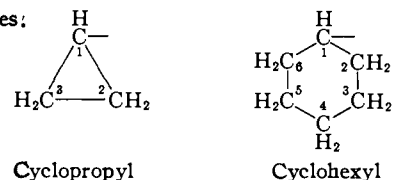
11.1.—The names of saturated monocyclic hydrocarbons (with no side chains) are formed by attaching the prefix "cyclo" to the name of the acyclic saturated unbranched hydrocarbon with the same number of carbon atoms. The generic name of saturated monocyclic hydrocarbons (with or without side chains) is "cycloalkane."

Examples:



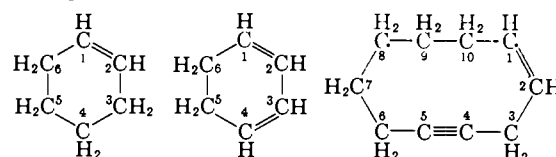
11.2.—Univalent radicals derived from cycloalkanes (with no side chains) are named by replacing the ending "-ane" of the hydrocarbon name by "-yl," the carbon atom with the free valence being numbered as 1. The generic name of these radicals is "cycloalkyl."

Examples:



11.3.—The names of unsaturated monocyclic hydrocarbons (with no side chains) are formed by substituting "-ene," "-adiene," "-atriene," "-yne," "-adiyne," *etc.*, for "-ane" in the name of the corresponding cycloalkane. The double and triple bonds are given numbers as low as possible as in Rule A-3.3.

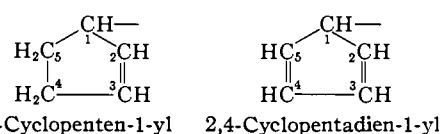
Examples:



The names "fulvene" (for methylenecyclopentadiene) and "benzene" are retained.

11.4.—The names of univalent radicals derived from unsaturated monocyclic hydrocarbons have the endings "-enyl," "-ynyl," "-dienyl," *etc.*, the positions of the double and triple bonds being indicated according to the principles of Rule A-3.3. The carbon atom with the free valence is numbered as 1, except as stated in the rules for terpenes (see Rules A-72 to A-75).

Examples:

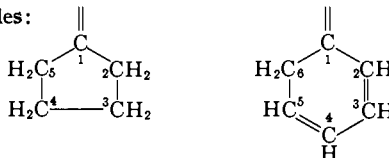


The radical name "phenyl" is retained.

◆ The point of attachment is numbered 1 and the double and triple bonds are given numbers as low as possible. The number 1 for the point of attachment is given in the radical name to emphasize the fact that the point of attachment takes precedence over the double and triple bonds (except with terpenes which have fixed numberings).

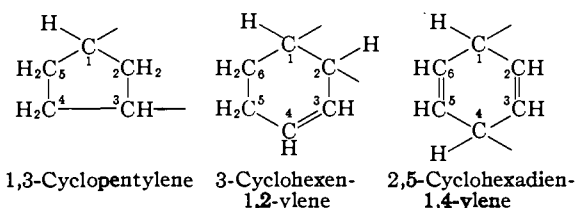
11.5.—Names of bivalent radicals derived from saturated or unsaturated monocyclic hydrocarbons by removal of two atoms of hydrogen from the same carbon atom of the ring are obtained by replacing the endings "-ane," "-ene," "-yne," by "-ylidene," "-enylidene" and "-ynylidene," respectively. The carbon atom with the free valences is numbered as 1, except as stated in the rules for terpenes.

Examples:

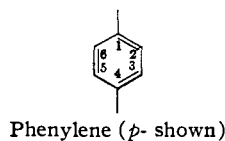


11.6.—Bivalent radicals derived from saturated or unsaturated monocyclic hydrocarbons by removing a hydrogen atom from each of two different carbon atoms of the ring are named by replacing the endings "-ane," "-ene," "-diene," "-yne," *etc.*, of the hydrocarbon name by "-ylene," "-enylene," "-dienylene," "-ynylene," *etc.*, the positions of the double and triple bonds and of the points of attachment being indicated. Preference in lowest numbers is given to the carbon atoms having the free valences.

Examples:

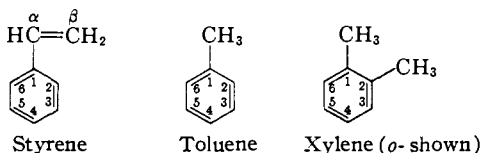
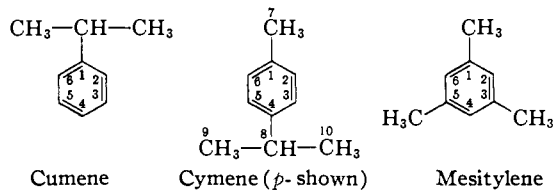


The name "phenylene" is retained



A-12

12.1.—These names for substituted monocyclic aromatic hydrocarbons are retained

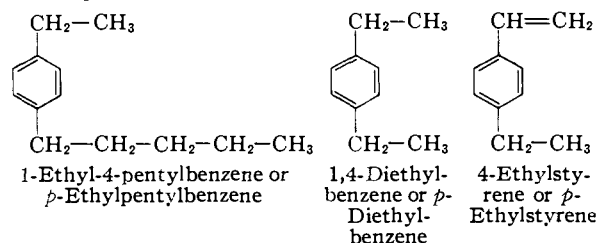


12.2.—Other substituted monocyclic aromatic hydrocarbons are named as derivatives of benzene or of one of the compounds listed in Part 1 of this rule. However, if the substituent introduced into such a compound is identical with one already present in that compound, then the substituted compound is named as a derivative of benzene (see Rule 61.4).

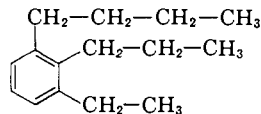
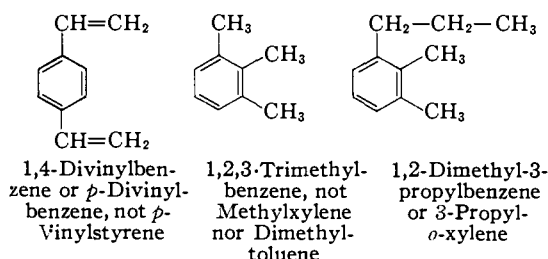
◆ *Chemical Abstracts* makes certain exceptions to the last part of this rule in order to favor a larger parent, although still treating like groups alike, *e.g.*, an *ar*-methyl derivative of cymene is indexed at Cumene, dimethyl-, not at Benzene, isopropylidimethyl-.

12.3.—The position of substituents is indicated by numbers except that *o*- (*ortho*-), *m*- (*meta*-) and *p*- (*para*-) may be used in place of 1,2-, 1,3-, and 1,4-, respectively, when only two substituents are present. The lowest numbers possible are given to substituents, choice between alternatives being governed by Rule A-2 so far as applicable, except that when names are based on those of compounds listed in Part 1 of this rule the first priority for lowest numbers is given to the substituent(s) already present in those compounds.

Examples:



◆ *Chemical Abstracts* limits the use of *o*-, *m*- and *p*- to like substituents when both are expressed as prefixes, *e.g.*, *p*-diethylbenzene, 1-ethyl-4-pentylbenzene. However, when one substituent is expressed in the name, *m*-, *o*- or *p*- is used to indicate the position of the second and different substituent, *e.g.*, *o*-ethylcumene.

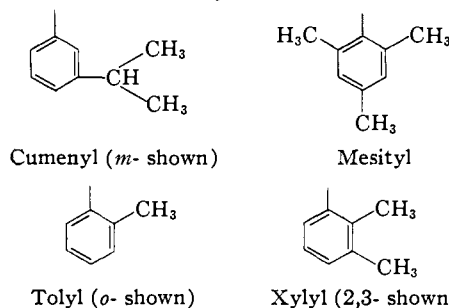


12.4.—The generic name of monocyclic and polycyclic aromatic hydrocarbons is "arene."

A-13

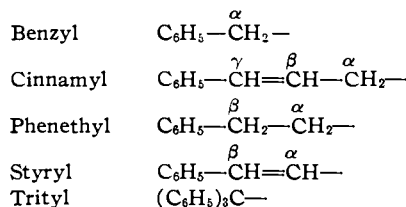
13.1.—Univalent radicals derived from monocyclic aromatic hydrocarbons and having the free valence at a ring atom are given the names listed below. Such radicals not listed below are named as substituted phenyl radicals. The carbon atom having the free valence is numbered as 1.

Phenyl C_6H_5-



13.2.—Since the name phenylene (*o*-, *m*- or *p*-) is retained for the radical $-C_6H_4-$ (exception to Rule A-11.6), bivalent radicals formed from substituted benzene derivatives and having the free valences at ring atoms are named as substituted phenylene radicals. The carbon atoms having the free valences are numbered 1,2-, 1,3- or 1,4- as appropriate.

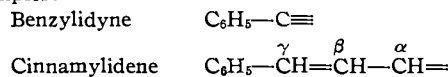
13.3.—These trivial names for radicals having a single free valence in the side chain are retained:



◆ *Chemical Abstracts* limits tryl to the unsubstituted radical.

13.4.—Multivalent radicals of aromatic hydrocarbons with the free valences in the side chain are named in accordance with Rule A-4.

Examples:



A-14

14.1.—The generic names of univalent and bivalent aromatic hydrocarbon radicals are "aryl" and "arylene," respectively.

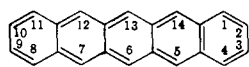
Fused Polycyclic Hydrocarbons

A-21

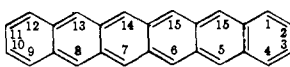
21.1.—The names of polycyclic hydrocarbons with maximum number of non-cumulative¹ double bonds end in "-ene." The names listed on pp. 5553 and 5554 are retained.

21.2.—The names of hydrocarbons containing five or more fused benzene rings in a straight linear arrangement are formed from a numerical prefix as specified in Rule A-1.1 followed by "-acene."

Examples:



Pentacene

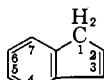


Hexacene

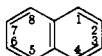
The following list contains the names of polycyclic hydrocarbons which are retained (see Rule A-21.1).



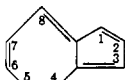
(1) Pentalene



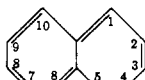
(2) Indene



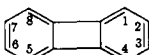
(3) Naphthalene



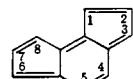
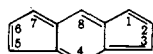
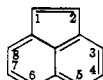
(4) Azulene



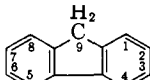
(5) Heptalene



(6) Biphenylene

(7) *as*-Indacene(8) *s*-Indacene

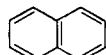
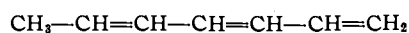
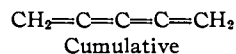
(9) Acenaphthylene



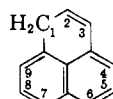
(10) Fluorene

(1) Cumulative double bonds are those present in a chain in which at least three contiguous carbon atoms are joined by double bonds; non-cumulative double bonds comprise every other arrangement of two or more double bonds in a single structure. The generic name "cumulene" is given to compounds containing three or more cumulative double bonds.

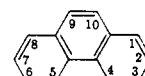
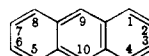
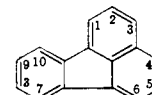
Examples:



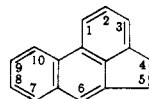
Non-cumulative



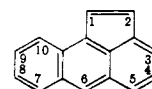
(11) Phenalene

(12) Phenanthrene¹(13) Anthracene¹

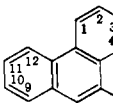
(14) Fluoranthene



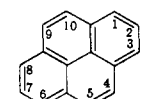
(15) Acephenanthrylene



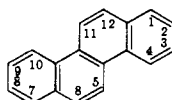
(16) Aceanthrylene



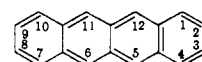
(17) Triphenylene



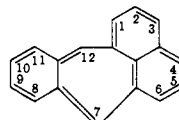
(18) Pyrene



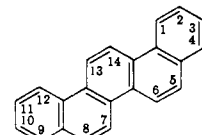
(19) Chrysene



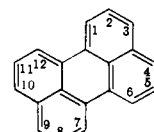
(20) Naphthacene



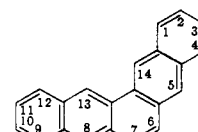
(21) Pleiadene



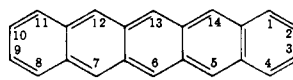
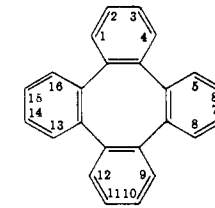
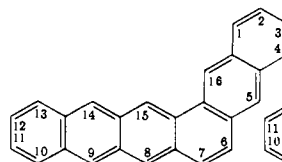
(22) Picene



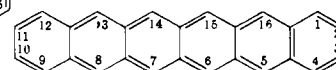
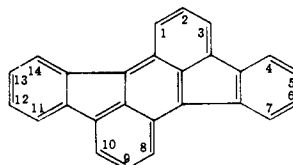
(23) Perylene



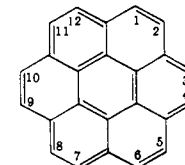
(24) Pentaphene

(25) Pentacene²(26) Tetraphenylene³

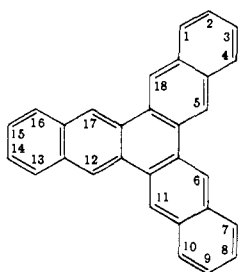
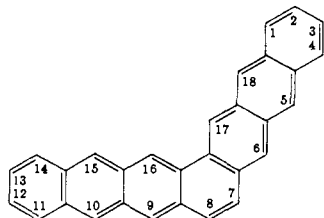
(27) Hexaphene

(28) Hexacene²

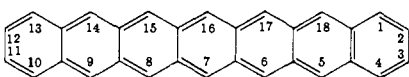
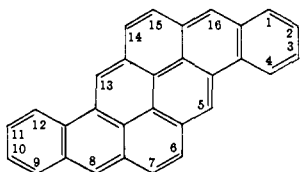
(29) Rubicene



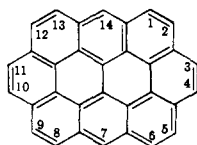
(30) Coronene

(31) Trinaphthylene^a

(32) Heptaphene

(33) Heptacene^a

(34) Pyranthrene



(35) Ovalene

(1) Denotes exception to systematic numbering. See Rule A-22.5.

(2) See Rule A-21.2.

(3) For isomer shown only.

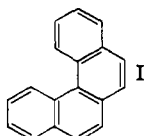
◆ Beginning with Volume 51 Subject Index *Chemical Abstracts* uses biphenylene in place of cyclobutadibenzene and phenalene in place of benzonaphthene. The polycyclic hydrocarbons which have the trivial names listed above may be used as the base components in naming orthofused or ortho- and peri-fused polycyclic systems for which there are no acceptable trivial names.

21.3.—“Ortho-fused”⁴ or “ortho- and peri-fused”⁵ polycyclic hydrocarbons with maximum number of non-cumulative double bonds which con-

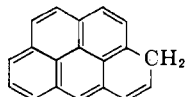
(4) Polycyclic compounds in which two rings have two, and only two, atoms in common are said to be “ortho-fused.” Such compounds have n common faces and $2n$ common atoms (Example I).

(5) Polycyclic compounds in which one ring contains two, and only two, atoms in common with each of two or more rings of a contiguous series of rings are said to be “ortho- and peri-fused.” Such compounds have n common faces and fewer than $2n$ common atoms (Examples II and III).

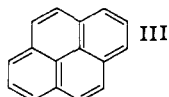
Examples:



3 common faces
6 common atoms
“Ortho-fused” system



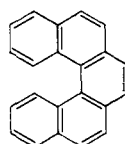
7 common faces
8 common atoms
“Ortho- and peri-fused” systems



5 common faces
6 common atoms
“Ortho- and peri-fused” systems

tain at least two rings of five or more members and which have no accepted trivial name such as those of 21.1 of this Rule, are named by prefixing to the name of a component ring or ring system (the base component) designations of the other components. The base component should contain as many rings as possible (provided it has a trivial name), and should occur as far as possible from the beginning of the list of Rule A-21.1. The attached components should be as simple as possible.

Example:



(not Naphthophenanthrene; benzo is “simpler” than naphtho, even though there are two benzo rings and only one naphtho)

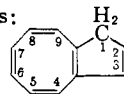
Dibenzophenanthrene

21.4.—The prefixes designating attached components are formed by changing the ending “-ene” of the name of the component hydrocarbon into “-eno,” e.g., “pyreno” (from pyrene). When more than one prefix is present, they are arranged in alphabetical order. These common abbreviated prefixes are recognized (see list in 21.1 of this Rule)

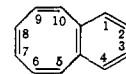
Acenaphtho	from	Acenaphthylene
Anthra	from	Anthracene
Benzo	from	Benzene
Naphtho	from	Naphthalene
Perylo	from	Perylene
Phenanthro	from	Phenanthrene

For monocyclic prefixes other than “benzo-” the following names are recognized, each to represent the form with the maximum number of non-cumulative double bonds: cyclopenta, cyclohepta, cycloocta, cyclonona, etc. When the base component is a monocyclic system, the ending “-ene” signifies the maximum number of non-cumulative double bonds, and does not denote one double bond only.

Examples:



1H-Cyclopentacyclooctene



Benzocyclooctene

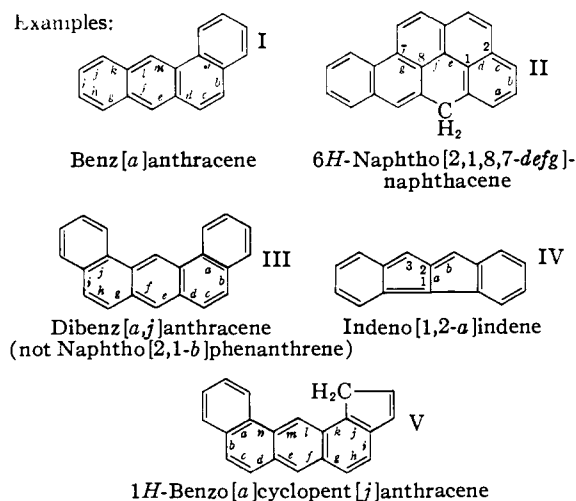
◆ In forming names of polycyclic systems from the above carbocyclic prefixes the final “o” or “a” of the prefix is elided before another vowel, except in the case of anthra, phenanthro and prefixes ending in -eno from which the “a” and “o” are never elided. Examples: benz[a]anthracene, cyclopent[a]acenaphthylene, anthra[1,2 - a]anthracene, fluoreno[4,3,2-de]anthracene.

The ending “-ene” to signify the maximum number of noncumulative double bonds in all fused carbocyclic systems means that the endings -diene, triene, tetraene, etc., are unnecessary when the base component is a monocyclic ring of seven or more carbon atoms. Higher stages of hydrogenation are indicated by the use of the prefixes dihydro-, tetrahydro-, etc. (cf. Rule A-23.1). *Chemical Abstracts* follows Rules A-21.4 and A-23.1 instead of Alternate Rule A-23.5.

21.5.—Isomers are distinguished by lettering the peripheral sides of the base component a , b , c , etc., beginning with “ a ” for the side “1,2,” “ b ” for “2,3” (or in certain cases “2,2a”) and lettering every side around the periphery. To the letter as early in the alphabet as possible, denoting the side where fusion occurs, are prefixed, if necessary, the numbers of the positions of attachment of the other component. These numbers are chosen to be as low as is con-

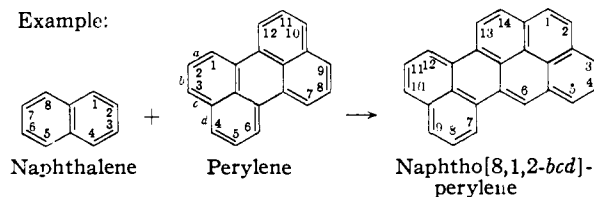
sistent with the numbering of the component, and their order conforms to the direction of lettering of the base component (see Examples II and IV). When two or more prefixes refer to equivalent positions so that there is a choice of letters, the prefixes are cited in alphabetical order according to Rule A-21.4 and the location of the first cited prefix is indicated by a letter as early as possible in the alphabet (see Example V). The numbers and letters are enclosed in brackets and placed immediately after the designation of the attached component. This expression merely defines the manner of fusion of the components.

Examples:



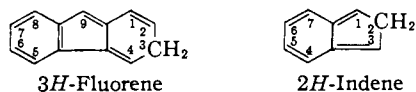
The completed system consisting of the base component and the other components is then renumbered according to Rule A-22, the numbering of the component parts being ignored.

Example:



21.6.—When a name applies equally to two or more isomeric condensed parent ring systems with the maximum number of non-cumulative double bonds and when the name can be made specific by indicating the position of one or more hydrogen atoms in the structure, this is accomplished by modifying the name with a locant, followed by italic capital *H* for each of these hydrogen atoms. Such symbols ordinarily precede the name. The said atom or atoms are called “indicated hydrogen.” The same principle is applied to radicals and compounds derived from these systems.

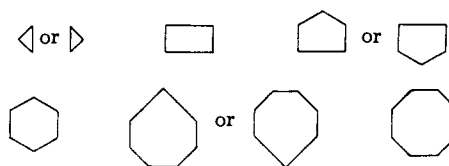
Examples:



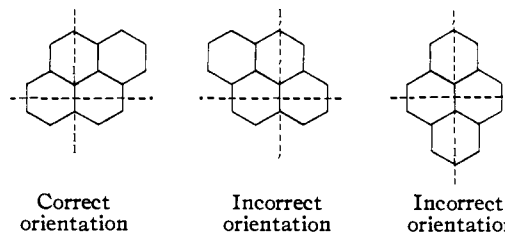
A-22

22.1.—For the purposes of numbering, the individual rings of a polycyclic “ortho-fused” or

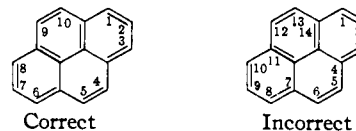
“ortho- and peri-fused” hydrocarbon system usually are drawn as follows:



and the polycyclic system is oriented so that (a) the greatest number of rings are in a horizontal row and (b) a maximum number of rings are above and to the right of the horizontal row (upper right quadrant). If two or more orientations meet these requirements, the one is chosen which has as few rings as possible in the lower left quadrant.

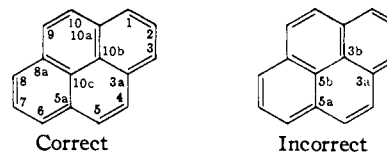


The system thus oriented is numbered in a clockwise direction commencing with the carbon atom not engaged in ring-fusion in the most counter-clockwise position of the uppermost ring, or if there is a choice, of the uppermost ring farthest to the right, and omitting atoms common to two or more rings.



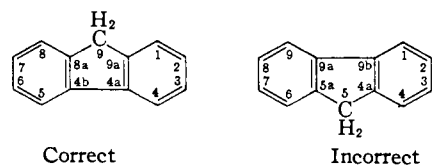
22.2.—Atoms common to two or more rings are designated by adding roman letters “a,” “b,” “c,” etc., to the number of the position immediately preceding. Interior atoms follow the highest number, taking a clockwise sequence wherever there is a choice.

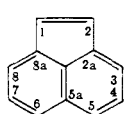
Examples: [cf. Note below]



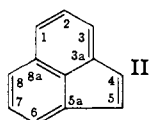
22.3.—When there is a choice, carbon atoms common to two or more rings follow the lowest possible numbers.

Examples:

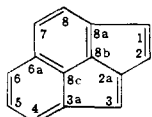




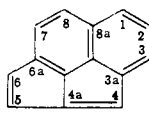
Correct



Incorrect



Correct



Incorrect

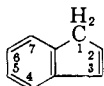
Note: I. 4, 4, 8, 9 is lower than 4, 5, 9, 9.

II. 2, 5, 8 is lower than 3, 5, 8.

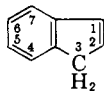
III. 2, 3, 6, 8 is lower than 3, 4, 6, 8 or 2, 4, 7, 8.

22.4.—When there is a choice, the carbon atoms which carry an indicated hydrogen atom are numbered as low as possible.

Examples:

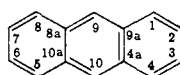


Correct

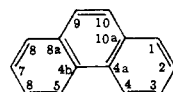


Incorrect

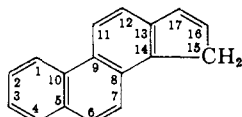
22.5.—The following are recommended exceptions to the above rules on numbering



Anthracene



Phenanthrene

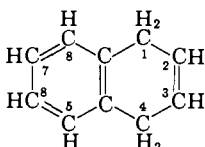
Cyclopenta [a]phenanthrene
(15*H*- shown)

See also rules on steroids

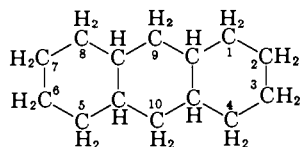
A-23

23.1.—The names of “ortho-fused” or “ortho- and peri-fused” polycyclic hydrocarbons with less than maximum number of non-cumulative double bonds are formed from a prefix “dihydro-,” “tetrahydro-,” *etc.*, followed by the name of the corresponding unreduced hydrocarbon. The prefix “perhydro-” signifies full hydrogenation. When there is a choice for *H* used for indicated hydrogen it is assigned the lowest available number.

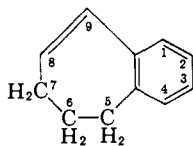
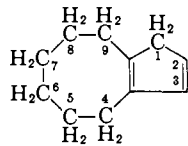
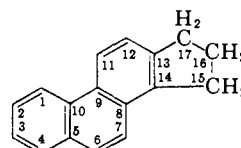
Examples:



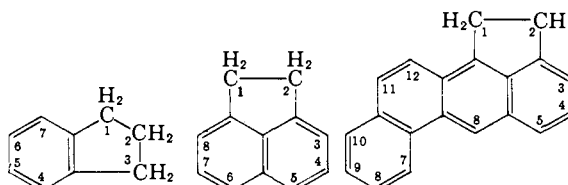
1,4-Dihydronaphthalene



Perhydroanthracene

6,7-Dihydro-5*H*-benzo-
cycloheptene4,5,6,7,8,9-Hexahydro-
1*H*-cyclopentacyclooctene16,17-Dihydro-15*H*-cyclopenta [a]phenanthrene

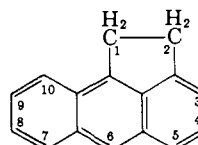
Exceptions: These names are retained



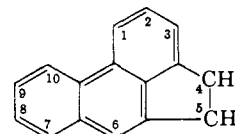
Indan

Acenaphthene

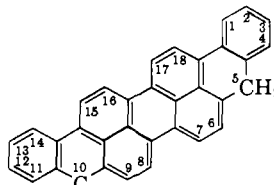
Cholanthrene



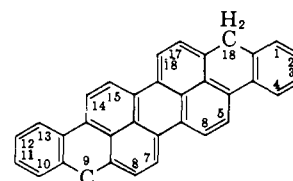
Aceanthrene



Acephenanthrene



Violanthrene

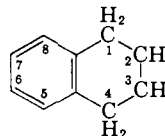


Isoviolanthrene

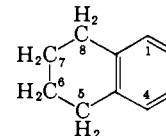
◆ *Chemical Abstracts* follows this Rule instead of the alternate Rule 23.5.

23.2.—When there is a choice, the carbon atoms to which hydrogen atoms are added are numbered as low as possible.

Example:



Correct

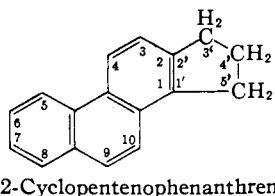
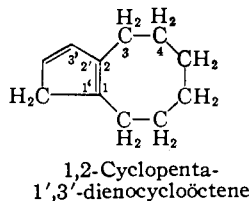
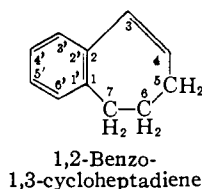


Incorrect

23.3.—Substituted polycyclic hydrocarbons are named according to the same principles as substituted monocyclic hydrocarbons (see Rules A-12 and A-61).

23.5 (Alternate to part of Rule A-23.1).—The names of “ortho-fused” polycyclic hydrocarbons which have (a) less than the maximum number of non-cumulative double bonds, (b) at least one terminal unit which is most conveniently named as an unsaturated cycloalkane derivative, and (c) a double bond at the positions where rings are fused together, may be derived by joining the name of the terminal unit to that of the other component by means of a letter “o” with elision of a terminal “e.” The abbreviations for fused aromatic systems laid down in Rule A-21.4 are used, and the exceptions of Rule A-23.1 apply.

Examples:



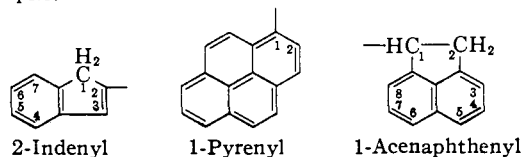
◆ *Chemical Abstracts* follows Rules A-21.4 and A-23.1 instead of this alternate rule.

A-24

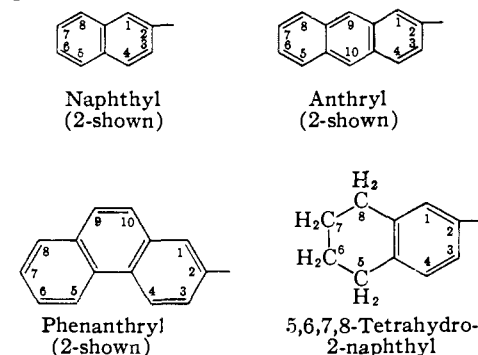
24.1.—For radicals derived from polycyclic hydrocarbons, the numbering of the hydrocarbon is retained. The point or points of attachment are given numbers as low as is consistent with the fixed numbering of the hydrocarbon.

24.2.—Univalent radicals derived from "ortho-fused" or "ortho- and peri-fused" polycyclic hydrocarbons with names ending in "-ene" by removal of a hydrogen atom from an aromatic or alicyclic ring are named in principle by changing the ending "-ene" of the names of the hydrocarbons to "-enyl."

Examples:



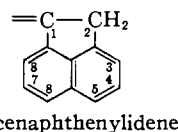
Exceptions:



◆ The above exceptions are limited to the simple rings as shown. Radicals from names of fused derivatives of these rings are formed according to the Rule, e.g., benz[*a*]anthracenyl.

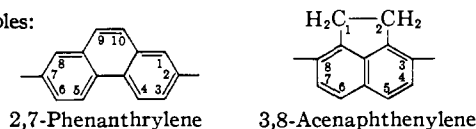
24.3.—Bivalent radicals derived from univalent polycyclic hydrocarbon radicals whose names end in "-yl" by removal of one hydrogen atom from the carbon atom with the free valence are named by adding "-idene" to the name of the corresponding univalent radical.

Example:



24.4.—Bivalent radicals derived from "ortho-fused" or "ortho- and peri-fused" polycyclic hydrocarbons by removal of a hydrogen atom from each of two different carbon atoms of the ring are named by changing the ending "-yl" of the univalent radical name to "-ylene."

Examples:



◆ *Chemical Abstracts* names multivalent radicals with three or more free valences derived from polycyclic hydrocarbons by an extension of Rule B-5.13 to carbocyclic systems. Example: 1,4,5-anthracenetriyl.

A-28

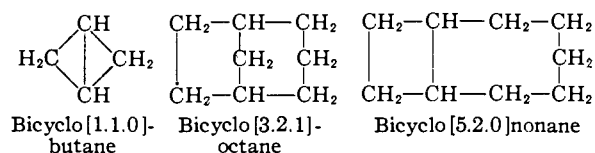
28.1.—Radicals formed from hydrocarbons consisting of polycyclic systems and side chains are named according to the principles of the preceding rules.

Bridged Hydrocarbons

A-31. von Baeyer System

31.1.—Saturated alicyclic hydrocarbon systems consisting of two rings only, having two or more atoms in common, take the name of an open chain hydrocarbon containing the same total number of carbon atoms preceded by the prefix "bicyclo-." The number of carbon atoms in each of the three bridges¹ connecting the two tertiary carbon atoms is indicated in brackets in descending order.

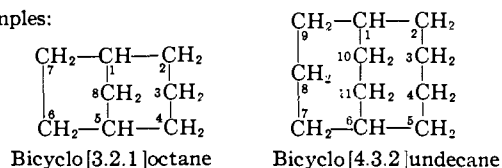
Examples:



(1) A bridge is a valence bond or an atom or an unbranched chain of atoms connecting two different parts of a molecule. The two tertiary carbon atoms connected through the bridge are termed "bridge-heads."

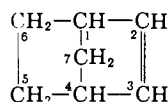
31.2.—The system is numbered commencing with one of the bridge-heads, numbering proceeding by the longest possible path to the second bridge-head; numbering is then continued from this atom by the longer unnumbered path back to the first bridge-head and is completed by the shortest path.

Examples:



Note: Longest path 1, 2, 3, 4, 5
Next longest path 5, 6, 7, 1
Shortest path 1, 8, 5

31.3.—Unsaturated hydrocarbons are named in accordance with the principles set forth in Rule A-11.3. When there is a choice in numbering unsaturation is given the lowest numbers.

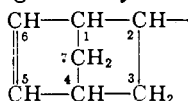


Bicyclo[2.2.1]hept-2-ene

◆ *Chemical Abstracts* names the above ring system 2-norbornene by Rule A-74.2, but follows the above Rule for hydrocarbons which do not have terpene names.

31.4.—Radicals derived from these hydrocarbons are named in accordance with the principles set forth in Rule A-11.4. The numbering of the hydrocarbon is retained and the point or points of attachment are given numbers as low as is consistent with the fixed numbering of the hydrocarbon.

Example:



Bicyclo[2.2.1]hept-5-en-2-yl

◆ *Chemical Abstracts* names the above radical 5-norbornen-2-yl by Rule A-75.2, but follows the above Rule for radicals derived from hydrocarbons which do not have terpene names. Radicals derived from the saturated hydrocarbons (except terpenes) are named by replacing the ending “-ane” of the hydrocarbon name by “-yl.” The point of attachment is given a number as low as is consistent with the fixed numbering of the hydrocarbon.

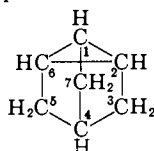
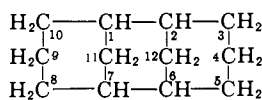
A-32

32.11.—Cyclic hydrocarbon systems consisting of three or more rings may be named in accordance with the principles stated in Rule A-31. The appropriate prefix “tricyclo-,” “tetracyclo-,” etc., is substituted for “bicyclo-” before the name of the open-chain hydrocarbon containing the same total number of carbon atoms.

32.12.—A polycyclic system is regarded as containing a number of rings equal to the number of scissions required to convert the system into an open-chain compound.

32.13.—The word “cyclo” is followed by brackets containing, in decreasing order, numbers indicating the number of carbon atoms in: the two branches of the main ring, the main bridge, the secondary bridges.

Examples:

Tricyclo[2.2.1.0⁴]heptaneTricyclo[5.3.1.1¹]dodecane

(1) For location and numbering of the secondary bridge see Rules A-32.22, A-32.23, A-32.31.

32.21.—The main ring and the main bridge form a bicyclic system whose numbering is made in compliance with Rule A-31.

32.22.—The location of the other or so-called secondary bridges is shown by superscripts following the number indicating the number of carbon atoms in the said bridges.

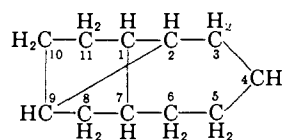
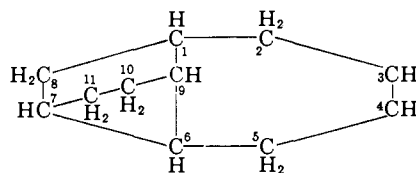
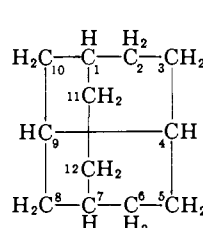
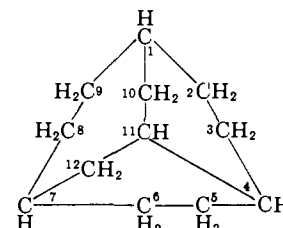
32.23.—For the purpose of numbering, the secondary bridges are considered in decreasing

order. The numbering of any bridge follows from the part already numbered, proceeding from the highest-numbered bridge-head.

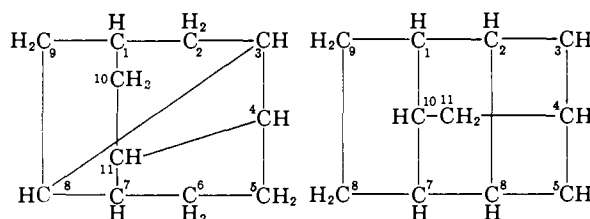
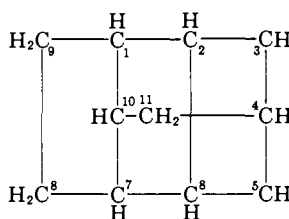
◆ Numbering of the secondary bridges by proceeding from the highest-numbered bridge-head of each bridge is an improvement over the former practice of “following the shortest path from the highest previous number.”

32.31.—When there is a choice, the following criteria are considered in turn until a decision is made:

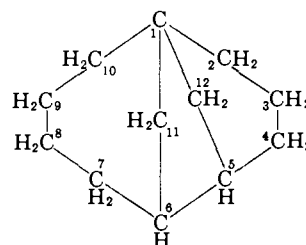
(a) The main ring shall contain as many carbon atoms as possible, two of which must serve as bridge-heads for the main bridge.

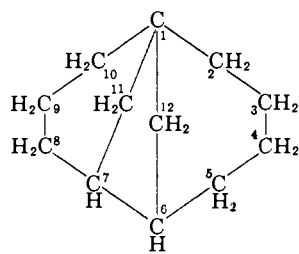
Tricyclo[5.4.0.0^{2,9}]undecane
Correct numberingTricyclo[4.2.1.2^{7,9}]undecane
Incorrect numberingTricyclo[5.3.2.0^{4,9}]dodecane
Correct numberingTricyclo[5.2.3.0^{4,11}]dodecane
Incorrect numbering

(b) The main bridge shall be as large as possible.

Tetracyclo[5.2.2.0^{3,8,0^4,11}]-undecane
Correct numberingTetracyclo[5.2.1.1^{4,10,0^2,6}]-undecane
Incorrect numbering

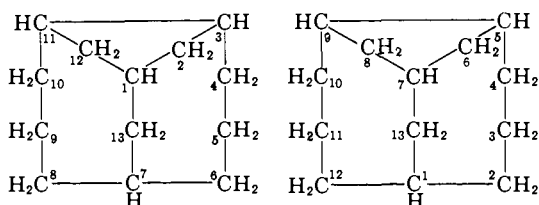
(c) The main ring shall be divided as symmetrically as possible by the main bridge.

Tricyclo[4.4.1.1⁸]dodecane:
Correct numbering



Tricyclo[5.3.1.1^{1,6}]dodecane:
Incorrect numbering

(d) The superscripts locating the other bridges shall be as small as possible (in the sense indicated in Rule A-2.2).



Tricyclo[5.5.1.0^{3,11}]tridecane
Correct numbering

Tricyclo[5.5.1.0^{6,9}]tridecane
Incorrect numbering

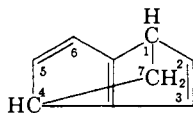
A-34 (Alternate to Rule A-35)

34.1.—Polycyclic hydrocarbon systems which can be regarded as “ortho-fused” or “ortho- and peri-fused” systems according to Rule A-21 and which, at the same time, have other bridges,¹ are first named as “ortho-fused” or “ortho- and peri-fused” systems. The other bridges are then indicated by prefixes derived from the corresponding hydrocarbon by replacing the final “-ane,” “-ene,” *etc.*, by “-ano,” “-eno,” *etc.*, and their positions are indicated by the points of attachment in the parent compound. If bridges of different types are present, they are cited in alphabetical order.

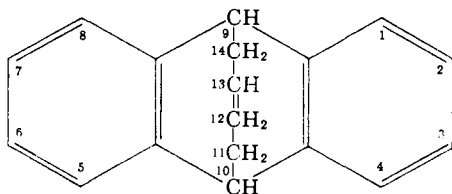
Examples of bridge names

Butano	—CH ₂ —CH ₂ —CH ₂ —CH ₂ —
Benzeno (<i>o</i> -, <i>m</i> -, <i>p</i> -)	—C ₆ H ₄ —
Ethano	—CH ₂ —CH ₂ —
Etheno	—CH=CH—
Methano	—CH ₂ —
Propano	—CH ₂ —CH ₂ —CH ₂ —

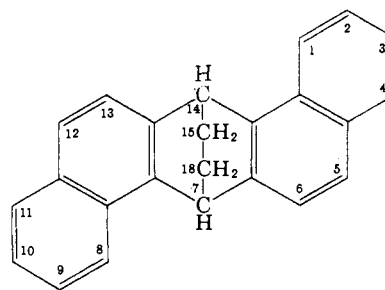
Examples:



1,4-Dihydro-1,4-
methanopentalene



9,10-Dihydro-9,10-(2-buten)-
anthracene

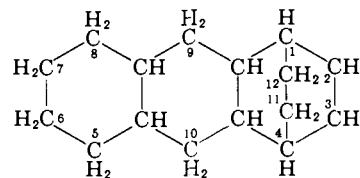


7,14-Dihydro-7,14-ethano-
dibenz[*a,h*]anthracene

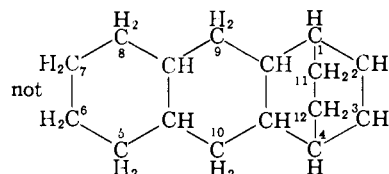
(1) The term “bridge,” when used in connection with an “ortho-fused” or “ortho- and peri-fused” polycyclic system as defined in note to Rule A-31.1, also includes “bivalent cyclic systems.”

34.2.—The parent “ortho-fused” or “ortho- and peri-fused” system is numbered as prescribed in Rule A-22. Where there is a choice, the position numbers of the bridge-heads should be as low as possible. The remaining bridges are then numbered in turn starting each time with the bridge atom next to the bridge-head possessing the highest number.

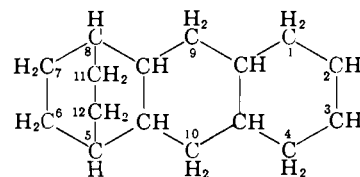
Example:



Perhydro-1,4-ethanoanthracene

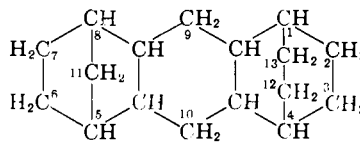


or



34.3.—When there is a choice of position numbers for the points of attachment for several individual bridges, the lowest numbers are assigned to the bridge-heads in the order of citation of the bridges and the bridge atoms are numbered according to the preceding rule.

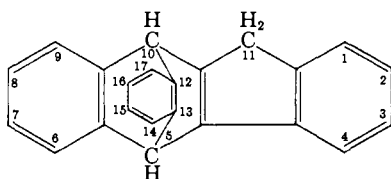
Example:



Perhydro-1,4-ethano-5,8-methanoanthracene

34.4.—When the bridge is formed from a bivalent cyclic hydrocarbon radical, low numbers are given to the carbon atoms constituting the shorter bridge and numbering proceeds around the ring.

Example:

10,11-Dihydro-5,10-*o*-benzo-5*H*-benzo[*b*]fluorene

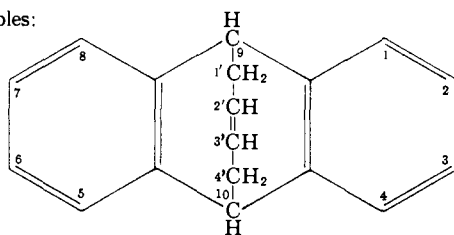
◆ *Chemical Abstracts* follows this rule instead of the Alternate Rule A-35.

A-35 (Alternate to Rule A-34)

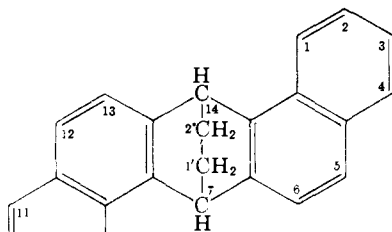
35.1.—Polycyclic hydrocarbons which can be regarded as “ortho-fused” or “ortho- and peri-fused” according to Rule A-21 and which have also other bridges may be named as “ortho-fused” or “ortho- and peri-fused” systems into which bivalent radicals are substituted.

35.2.—Compounds which are named in accordance with 35.1 of this rule are numbered as prescribed in Rule A-34. The bridge is numbered independently. Numbering of the bridge is started at the lower-numbered bridge-head. Numbers assigned to the bridge atoms are primed.

Examples:



9,10-Dihydro-9,10-(2'-butenyloxy)anthracene

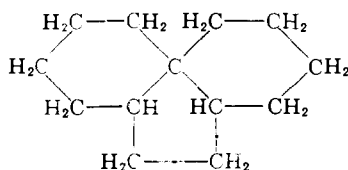
7,14-Dihydro-7,14-ethylene-dibenz[*a,h*]anthracene

◆ *Chemical Abstracts* follows Rule A-34 instead of this Alternate Rule.

Spiro Hydrocarbons

A “spiro union” is one formed by a single atom which is the only common member of two rings. A “free spiro union” is one constituting the only union direct or indirect between two rings.¹ The common atom is designated as the “spiro atom.” According to the number of spiro atoms present, the

(1) An example of a compound where the spiro union is not free is:

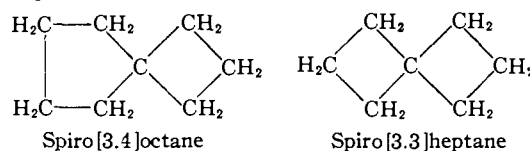


compounds are distinguished as monospiro, dispiro, trispiro compounds, *etc.* The following rules apply to the naming of compounds containing free spiro unions.

A-41 (Alternate to Rule A-42)

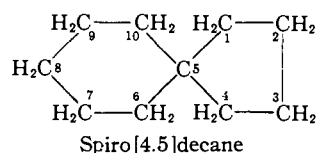
41.1.—Monospiro compounds consisting of only two alicyclic rings as components are named by placing “spiro” before the name of the normal acyclic hydrocarbon of the same total number of carbon atoms. The number of carbon atoms linked to the spiro atom in each ring is indicated in ascending order in brackets placed between the spiro prefix and the hydrocarbon name.

Examples:



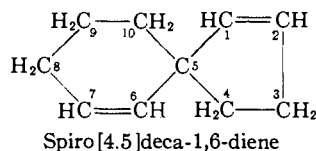
41.2.—The carbon atoms in monospiro hydrocarbons are numbered consecutively starting with a ring atom next to the spiro atom, first through the smaller ring (if such be present) and then through the spiro atom and around the second ring.

Example:



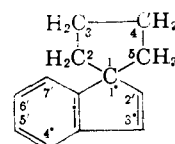
41.3.—When unsaturation is present, the same numbering pattern is maintained, but in such a direction around the rings that the double and triple bonds receive numbers as low as possible in accordance with Rule A-11.

Example:



41.4.—If one or both components of the monospiro compound are fused polycyclic systems, “spiro” is placed before the names of the components arranged in alphabetical order and enclosed in brackets. Established numbering of the individual components is retained. The lowest possible number is given to the spiro atom, and the numbers of the second component are marked with primes. The position of the spiro atom is indicated by placing the appropriate numbers between the names of the two components.

Example:

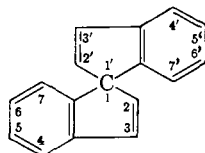


Spiro[cyclopentane-1,1'-indene]

41.5.—Monospiro compounds containing two similar polycyclic components are named by placing the prefix “spirobi” before the name of the compo-

nent ring system. Established numbering of the polycyclic system is maintained and the numbers of one component are distinguished by primes. The position of the spiro atom is indicated in the name of the spiro compound by placing the appropriate locants before the name.

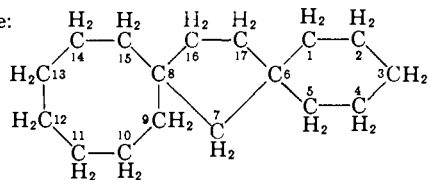
Example:



1,1'-Spirobiindene

41.6.—Polyspiro compounds consisting of three or more alicyclic systems are named by placing "dispiro," "trispiro," "tetraspiro," etc., before the name of the normal acyclic hydrocarbon of the same total number of carbon atoms. The numbers of carbon atoms linked to the spiro atoms in each ring are indicated in brackets in the same order as the numbering proceeds about the ring. Numbering starts with a ring atom next to a terminal spiro atom and proceeds in such a way as to give the spiro atoms as low numbers as possible.

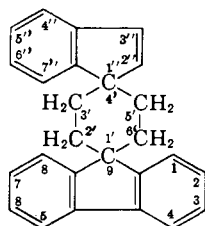
Example:



Dispiro[5.1.7.2]heptadecane

41.7.—Polycyclic compounds containing more than one spiro atom and at least one fused polycyclic component are named in accordance with 41.4 of this rule by replacing "spiro" with "dispiro," "trispiro," etc., and choosing the end components by alphabetical order.

Example:



Dispiro[fluorene-9,1'-cyclohexane-4',1''-indene]

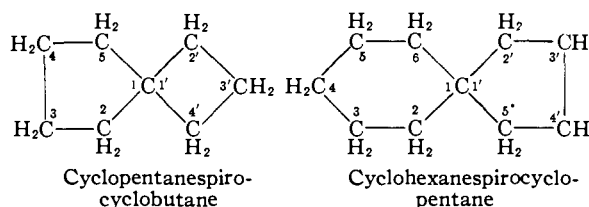
◆ This represents the method of naming spiro compounds which is followed by *Chemical Abstracts* instead of the Alternate Rule A-42.

A-42

42.1 (Alternate to A-41.1 and A-41.2).—When two dissimilar cyclic components are united by a spiro union, the name of the larger component is followed by the affix "spiro" which, in turn, is followed by the name of the smaller component. Between the affix "spiro" and the name of each component system is inserted the number denoting the spiro-position in the appropriate ring system, these numbers being as low as permitted by any fixed numbering of the component. The components retain their respective numberings but numbers for the component mentioned second are

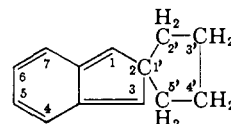
primed. Numbers 1 may be omitted when a free choice is available for a component.

Examples:



Cyclopentanespiro-cyclobutane

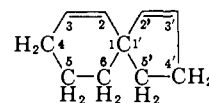
Cyclohexanespirocyclopentane



2H-Indene-2-spiro-1'-cyclopentane

42.2 (Alternate to A-41.3).—Rule A-41.3 applies also with appropriate different numbering where nomenclature is according to Rule A-42.1, but the spiro-union has priority for lowest numbers over unsaturation.

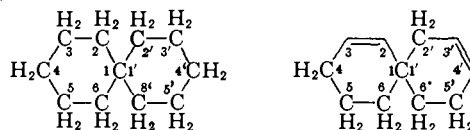
Example:



2-Cyclohexenespiro-(2'-cyclopentene)

42.3 (Alternate to A-41.5).—The nomenclature of Rule A-41.5 is applied also to monocyclic components with identical saturation, the spiro-union being numbered 1.

Examples:

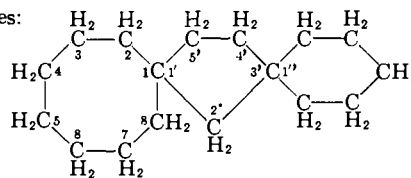


Spirobicyclohexane

but 2-Cyclohexenespiro-(3'-cyclohexene)

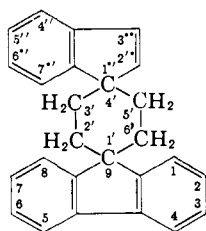
42.4 (Alternate to A-41.6 and A-41.7).—Polycyclic compounds containing more than one spiro atom are named in accordance with Rule A-42.1 starting from the senior¹ end-component irrespective of whether the components are simple or fused rings.

Examples:



Cyclooctanespirocyclopentane-3'-spirocyclohexane

(1) "Seniority" in respect to spiro compounds is based on the principles: (i) an aggregate is senior to a monocycle; (ii) of aggregates, the senior is that containing the largest number of individual rings; (iii) of aggregates containing the same number of individual rings, the senior is that containing the largest ring; (iv) if aggregates consist of equal number of equal rings the senior is the first occurring in the alphabetical list of names.



Fluorene-9-spiro-1'-cyclohexane-4'-spiro-1''-indene

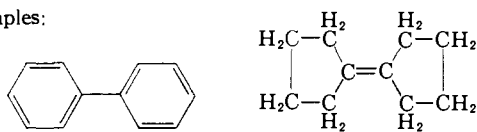
◆ *Chemical Abstracts* follows Rule A-41 instead of this Alternate Rule.

Hydrocarbon Ring Assemblies

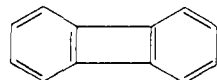
A-51

51.1.—Two or more cyclic systems (single rings or fused systems) which are directly joined to each other by double or single bonds are named “ring assemblies” when the number of such direct ring junctions is one less than the number of cyclic systems involved.

Examples:



Ring assemblies

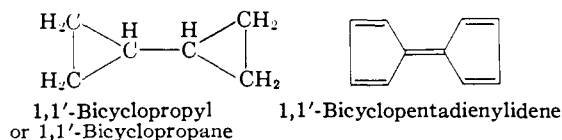


Fused polycyclic system

A-52

52.1.—Assemblies of two identical cyclic hydrocarbon systems are named in either of two ways: (a) by placing the prefix “bi-” before the name of the corresponding radical, or (b) for systems joined by a single bond by placing the prefix “bi-” before the name of the corresponding hydrocarbon. In each case, the numbering of the assembly is that of the corresponding radical or hydrocarbon, one system being assigned unprimed numbers and the other primed numbers. The points of attachment are indicated by placing the appropriate locants before the name.

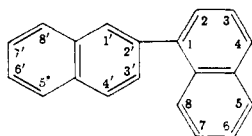
Examples:

1,1'-Bicyclopentadienyl
or 1,1'-Bicyclopentadiene

1,1'-Bicyclopentadienylidene

52.2.—If there is a choice in numbering, unprimed numbers are assigned to the system which has the lower-numbered point of attachment.

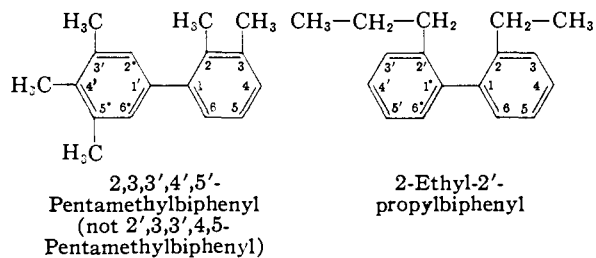
Example:

1,2'-Binaphthyl
or 1,2'-Binaphthalene

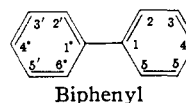
52.3.—If two identical hydrocarbon systems have the same point of attachment and contain substitu-

ents at different positions, the locants of these substituents are assigned according to Rule A-2.2; for this purpose an unprimed number is considered lower than the same number when primed. Assemblies of primed and unprimed numbers are arranged in ascending numerical order.

Examples:

2,3,3',4',5'-
Pentamethylbiphenyl
(not 2',3,3',4,5-
Pentamethylbiphenyl)2-Ethyl-2'-
propylbiphenyl

52.4.—The name “biphenyl” is used for the assembly consisting of two benzene rings.



Biphenyl

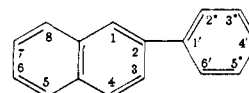
A-53

53.1.—Other hydrocarbon ring assemblies are named by selecting one ring system as the base component and considering the other systems as substituents of the base component. Such substituents are arranged in alphabetical order. The base component is assigned unprimed numbers and the substituents are assigned numbers with primes.

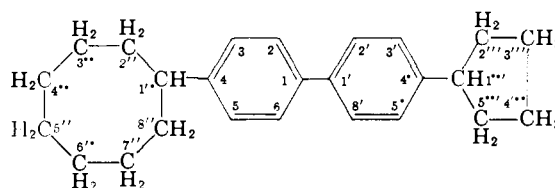
53.2.—The base component is chosen by considering these characteristics in turn until a decision is reached:

(a) The system containing the larger number of rings.

Examples:



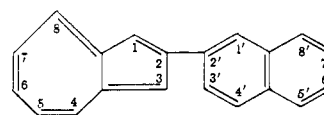
2-Phenylnaphthalene



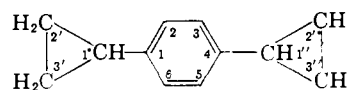
4-Cyclooctyl-4'-cyclopentylbiphenyl

(b) The system containing the larger ring.

Examples:

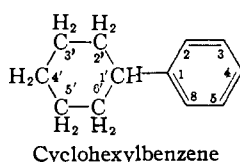


2-(2'-Naphthyl)azulene

1,4-Dicyclopropylbenzene
or *p*-Dicyclopropylbenzene

(c) The system in the lowest state of hydrogenation (see also 53.3 of this rule).

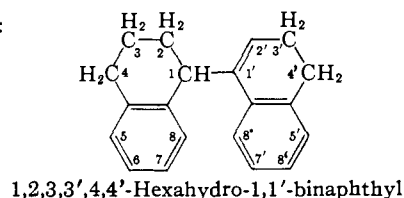
Example:



(d) The order of ring systems as set forth in the list of Rule A-21.1.

53.3.—Compounds covered by 53.2(c) of this rule may also be named as hydrogenation products according to Rule A-23.

Example:



◆ The name of the second example in (a) which contains as a base component the ring assembly "biphenyl" indicates that the word system as used here includes ring assemblies as base components.

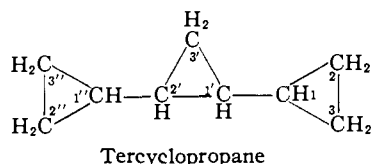
Chemical Abstracts does not use primed numbers with the groups which may be considered as substituent groups expressed as prefixes and attached to the name of the base component. Examples: 2-(2,4-dichlorophenyl)naphthalene; 2-(2-naphthyl)azulene.

A-54

54.1.—Unbranched assemblies consisting of three or more identical hydrocarbon ring systems are named by placing an appropriate numerical prefix before the name of the hydrocarbon corresponding to the repetitive unit. These numerical prefixes are used:

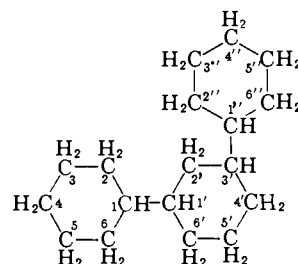
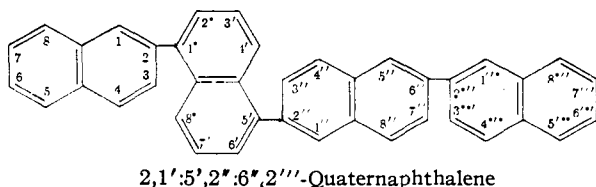
3. ter-	7. septi-
4. quater-	8. octi-
5. quinque-	9. novi-
6. sexi-	10. deci-

Example:



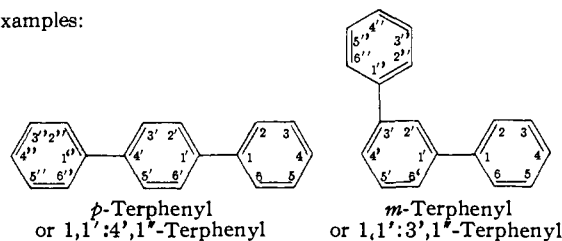
54.2.—Unprimed numbers are assigned to one of the terminal systems, the other systems being primed serially. Points of attachment are assigned the lowest numbers possible.

Examples:



54.3.—As exceptions, unbranched assemblies consisting of benzene rings are named by using the appropriate prefix with the radical name "phenyl."

Examples:



Cyclic Hydrocarbons with Side Chains

(Note: *cf.* Rules A-12 and A-13)

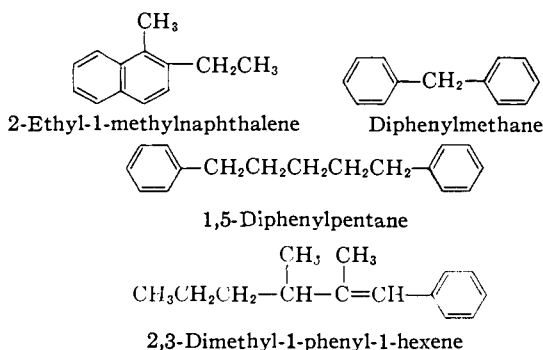
A-61

61.1.—Hydrocarbons more complex than those envisioned in Rule A-12, composed of cyclic nuclei and aliphatic chains, are named according to one of the methods given below. Choice is made so as to provide the name which is the simplest permissible or the most appropriate for the chemical intent.

61.2.—When there is no generally recognized trivial name for the hydrocarbon, then (1) the radical name denoting the aliphatic chain is prefixed to the name of the cyclic hydrocarbon, or (2) the radical name for the cyclic hydrocarbon is prefixed to the name of the aliphatic compound. Choice between these methods is made according to the more appropriate of the following principles: (a) the maximum number of substitutions into a single unit of structure; (b) treatment of a smaller unit of structure as a substituent into a larger.

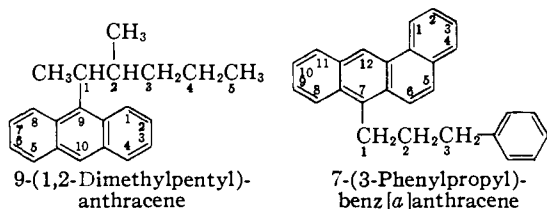
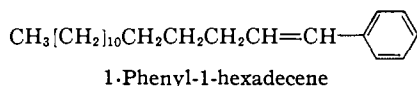
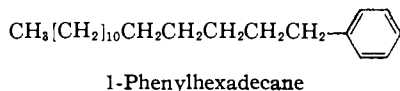
61.3.—In accordance with the principle (a) of 61.2 of this rule, hydrocarbons containing several chains attached to one cyclic nucleus generally are named as derivatives of the cyclic compound; and compounds containing several side chains and/or cyclic radicals attached to one chain are named as derivatives of the acyclic compound.

Examples:



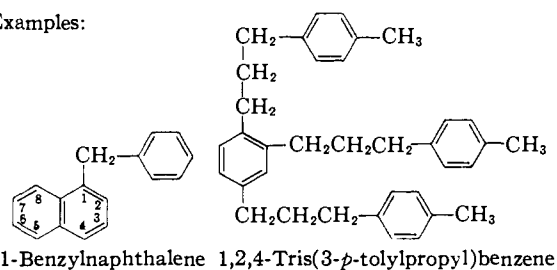
61.4.—In accordance with principle (b) of 61.2 of this rule, a hydrocarbon containing a small cyclic nucleus attached to a long chain is generally named as a derivative of the acyclic hydrocarbon; and a hydrocarbon containing a small group attached to a large cyclic nucleus is generally named as a derivative of the cyclic hydrocarbon.

Examples:



61.5.—Recognized trivial names for composite radicals are used if they lead to simplifications in naming.

Examples:



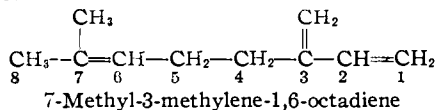
Terpene Hydrocarbons

Owing to long-established custom, terpenes are given exceptional treatment in these rules.

A-71. Acyclic Terpenes¹

71.1.—The acyclic terpene hydrocarbons are named in a manner similar to that used for other unsaturated acyclic hydrocarbons when pure compounds are involved.

Example:



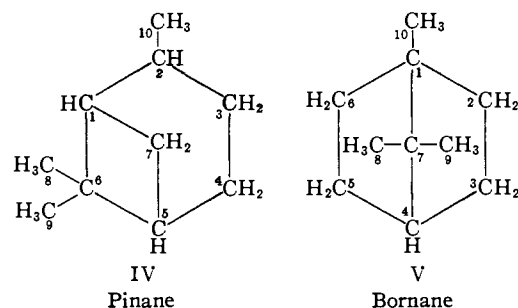
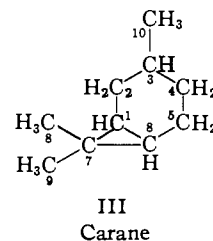
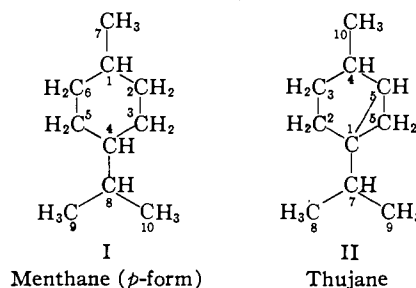
A-72. Cyclic Terpenes

72.1.—The following structural types with their special names and special systems of numbering are used as the basis for the specialized nomenclature of monocyclic and bicyclic terpene hydrocarbons. The name "bornane" replaces camphane

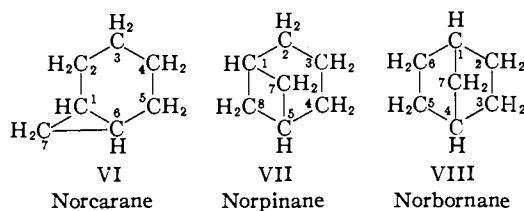
(1) For a more complete discussion of terpene nomenclature see "Nomenclature for Terpene Hydrocarbons," Advances in Chemistry Series No. 14 (American Chemical Society).

and bornylane; "norbornane" replaces norcamphane and norbornylane.

Fundamental terpene types:



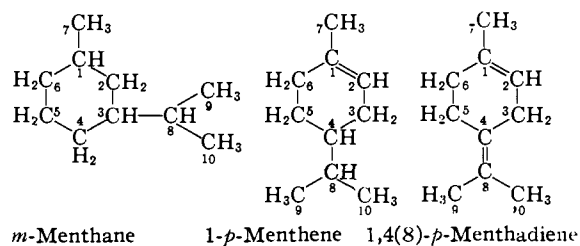
Nor-structures:



A-73. Monocyclic Terpenes

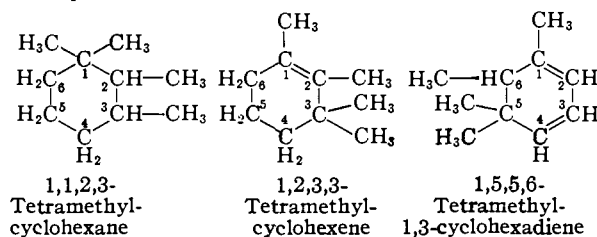
73.1.—Menthane Type: Monocyclic terpene hydrocarbons of this type (ortho, meta, and para isomers) are named menthane, menthene, menthadiene, etc., and are given the fixed numbering of menthane (Formula I). Such compounds substituted by additional alkyl groups are named in accordance with Rule A-11.

Examples:



73.2.—Tetramethylcyclohexane Type: Monocyclic terpene hydrocarbons of this type are named systematically as derivatives of cyclohexane, cyclohexene, and cyclohexadiene (see Rule A-11).

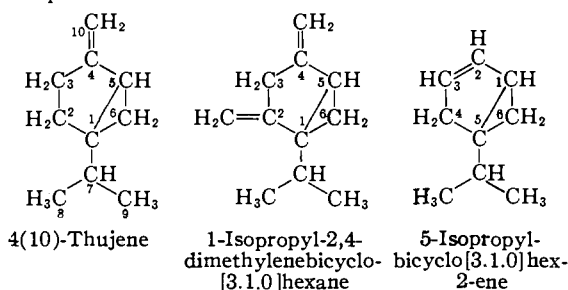
Examples:



A-74. Bicyclic Terpenes

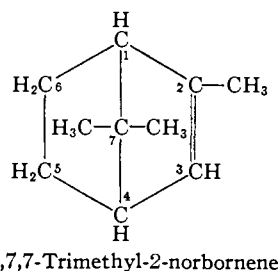
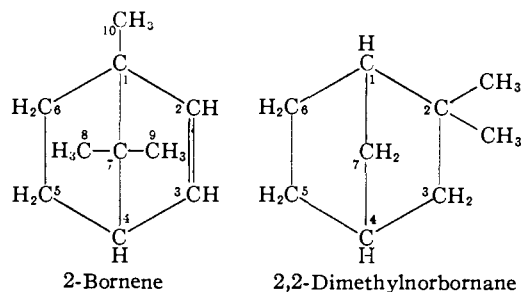
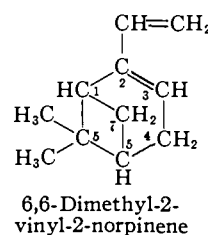
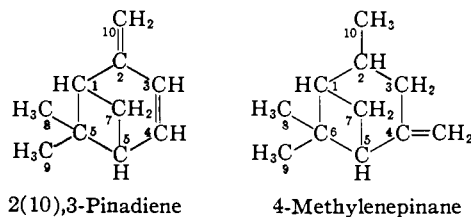
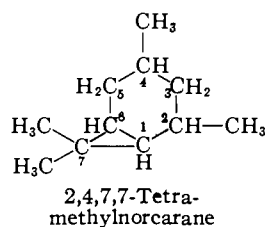
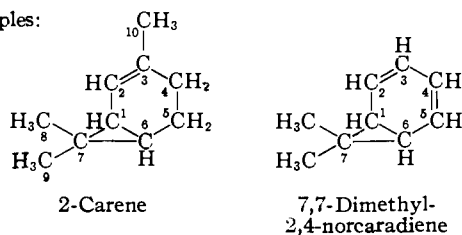
74.1.—Bicyclic terpene hydrocarbons having the skeleton of Formula II or this skeleton and additional side chains except methyl or isopropyl (or methylene if one methylene group is already present) are named as thujane, thujene, thujadiene, etc., and are given the fixed numbering shown for thujane (Formula II). Other hydrocarbons containing the thujane ring-skeleton are named from bicyclo[3.1.0]hexane and are given systematic bicyclo numbering (cf. Rule A-31).

Examples:

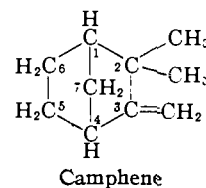


74.2.—Bicyclic terpene hydrocarbons having the skeleton of Formula III, IV, or V and additional side chains except methyl (or methylene if one methylene group is already present) are named, respectively, as carane, carene, caradiene, etc.; pinane, pinene, pinadiene, etc.; bornane, bornene, bornadiene, etc. They are given, respectively, the fixed numbering shown for carane (Formula III), pinane (Formula IV), and bornane (Formula V). Other hydrocarbons containing the ring-skeleton of carane, pinane, or bornane are named, respectively, from norcarane (Formula VI), norpinane (Formula VII), or norbornane (Formula VIII). These names are preferred to those from bicyclo[4.1.0]heptane, bicyclo[3.1.1]heptane, or bicyclo[2.2.1]heptane. The nor-names are given systematic bicyclo numbering (cf. Rule A-31).

Examples:



74.3.—The name "camphene" is retained for the unsubstituted compound 2,2-dimethyl-3-methylenenorbornane.

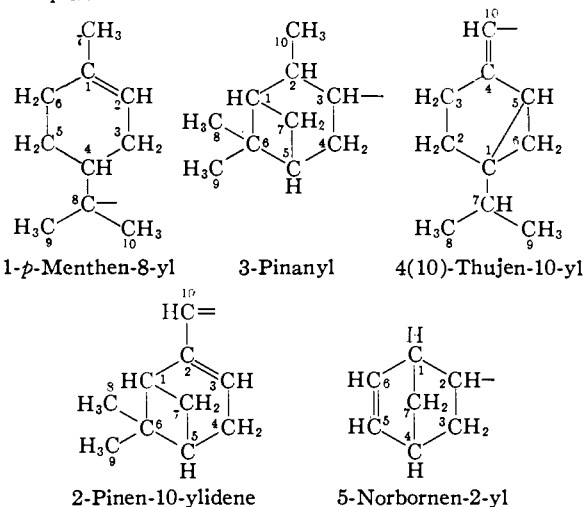


A-75. Terpene Radicals

75.1.—Simple acyclic hydrocarbon terpene radicals are named and numbered according to Rule A-3.5. The trivial names geranyl, neryl, linalyl and phytyl are retained for the unsubstituted radicals.

75.2.—Radicals derived from menthane, pinane, thujane, carane, bornane, norcarane, norpinane, and norbornane are named in accordance with the principles set forth in Rules A-1.2 and A-11.4 except that the saturated radicals of pinane are named pinanyl, pinanylene, and pinanylidene. The numbering of the hydrocarbon is retained and the point or points of attachment, whether in the ring or side chain, are given numbers as low as is consistent with the fixed numbering of the hydrocarbon.

Examples:



75.3.—Radicals not named in Rules A-75.1 and A-75.2 are named as described in Rules A-11 and A-31.4.

B. FUNDAMENTAL HETEROCYCLIC SYSTEMS

B-1. Extension of Hantzsch-Widman System

1.1.—Monocyclic compounds containing one or more hetero atoms in a three- to ten-membered ring are named by combining the appropriate prefix or prefixes from Table I (eliding "a" where necessary) with a stem from Table II. The state of hydrogenation is indicated either in the stem, as shown in Table II, or by the prefixes "dihydro-," "tetrahydro-," etc., according to Rule B-1.2.

Element	Valence	Prefix
Oxygen	II	Oxa
Sulfur	II	Thia
Selenium	II	Selena
Tellurium	II	Tellura
Nitrogen	III	Aza
Phosphorus	III	Phospha ^a
Arsenic	III	Arsa ^a
Antimony	III	Stiba ^a
Bismuth	III	Bisma
Silicon	IV	Sila
Germanium	IV	Germa
Tin	IV	Stanna
Lead	IV	Plumba
Mercury	II	Mercura

^a When immediately followed by "-in" or "-ine," "phospha-" should be replaced by "phosphor-," "arsa-" should be replaced by "arsen-" and "stiba" should be replaced by "antimon-."

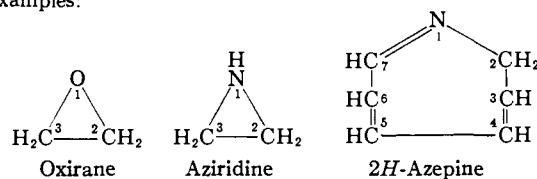
◆ "Bora" for boron is used frequently. *Chemical Abstracts* has placed boron with the valence of III between lead and mercury in Table I. This table shows the valence of tin and lead as IV instead of II (a correction of a typographical error).

TABLE II

No. of members in the ring	Rings containing nitrogen		Rings containing no nitrogen	
	Unsaturation ^a	Saturation	Unsaturation ^a	Saturation
3	-irine	-iridine	-irene	-irane ^e
4	-ete	-etidine	-ete	-etane
5	-ole	-olidine	-ole	-olane
6	-ine ^b	"	-in ^b	-ane ^d
7	-epine	"	-epin	-epane
8	-ocine	"	-ocin	-ocane
9	-onine	"	-onin	-onane
10	-ecine	"	-ecin	-ecane

^a Corresponding to the maximum number of non-cumulative double bonds, the hetero elements having the normal valences shown in Table I. ^b For phosphorus, arsenic, antimony, see the special provisions of Table I. ^c Expressed by prefixing "perhydro" to the name of the corresponding unsaturated compound. ^d Not applicable to silicon, germanium, tin and lead. In this case, "perhydro-" is prefixed to the name of the corresponding unsaturated compound. ^e The syllables denoting the size of rings containing 3, 4 or 7-10 members are derived as follows: "ir" from *tri*-, "et" from *tetra*-, "ep" from *hepta*-, "oc" from *octa*-, "on" from *nona*-, and "ec" from *deca*.

Examples:

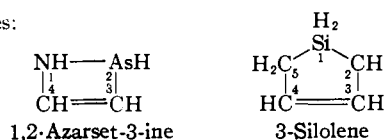


1.2.—Heterocyclic systems whose unsaturation is less than the one corresponding to the maximum number of noncumulative double bonds are named by using the prefixes "dihydro-," "tetrahydro-," etc.

In the case of 4- and 5-membered rings, a special termination is used for the structures containing one double bond, when there can be more than one non-cumulative double bond.

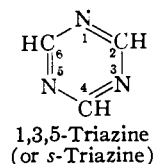
No. of members of the partly saturated rings	Rings containing nitrogen	Rings containing no nitrogen
4	-etine	-etene
5	-oline	-olene

Examples:



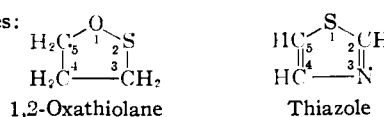
1.3.—Multiplicity of the same hetero atom is indicated by a prefix "di-," "tri-," etc., placed before the appropriate "a" term (Table I).

Example:



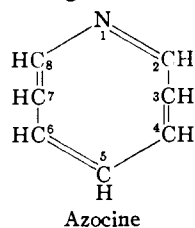
1.4.—If two or more kinds of "a" terms occur in the same name, their order of citation is by descending group number of the Periodic Table and increasing atomic number in the group as illustrated by the sequence in Table I.

Examples:



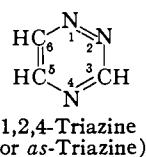
1.51.—The position of a single hetero atom determines the numbering in a monocyclic compound.

Example:



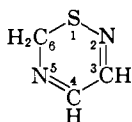
1.52.—When the same hetero atom occurs more than once in a ring, the numbering is chosen to give the lowest locants to the hetero atoms.

Example:

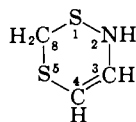


1.53.—When hetero atoms of different kinds are present, the locant 1 is given to a hetero atom which is as high as possible in Table I. The numbering is then chosen to give the lowest locants to the hetero atoms.

Examples:



6*H*-1,2,5-Thiadiazine
(not 2,1,4-Thiadiazine)
(not 1,3,6-Thiadiazine)



2*H*,6*H*-1,5,2-Dithiazine
(not 1,3,4-Dithiazine)
(not 1,3,6-Dithiazine)
(not 1,5,4-Dithiazine)

The numbering must begin with the sulfur atom. This condition eliminates 2,1,4-thiadiazine. Then the nitrogen atoms receive the lowest possible locant, which eliminates 1,3,6-thiadiazine.

The numbering must begin with a sulfur atom. The choice of this atom is determined by the set of locants which can be attributed to the remaining hetero atoms of any kind. As the set 1,2,5 is lower than 1,3,4 or 1,3,6 or 1,5,4 in the usual sense, the name is 1,5,2-dithiazine.



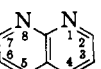
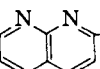


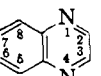
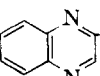
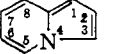
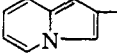
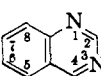
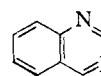
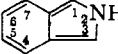
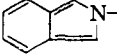
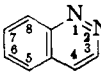
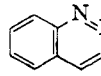
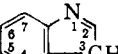
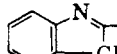
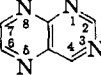
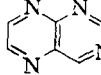
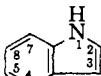
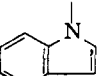
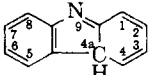
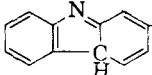
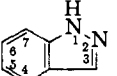
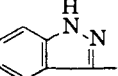
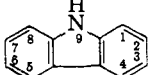
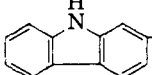
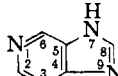
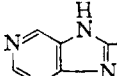
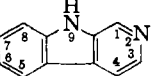
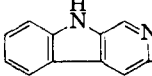
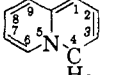
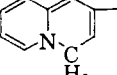
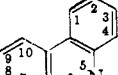
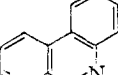
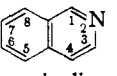
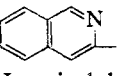
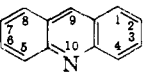
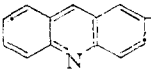
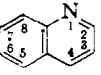
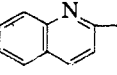
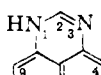
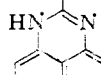
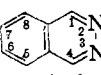
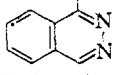
B-2. Trivial and Semi-trivial Names

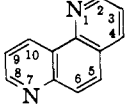
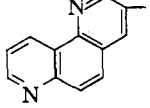
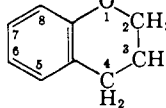
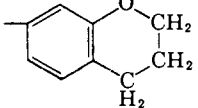
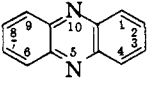
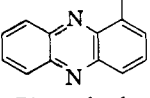
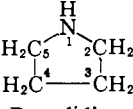
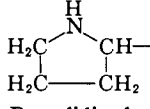
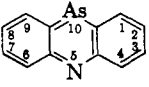
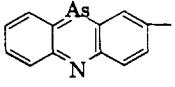
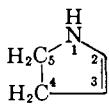
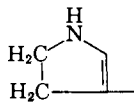


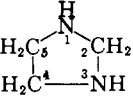
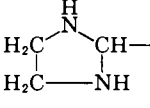
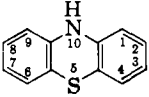
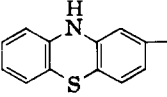
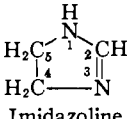
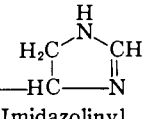


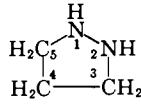
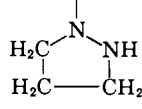


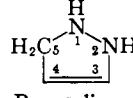
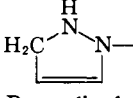
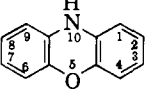
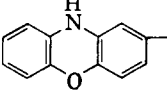
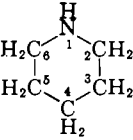
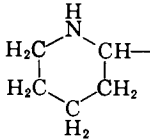
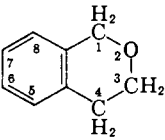
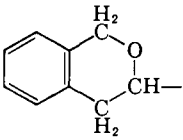
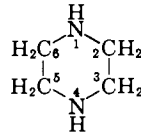
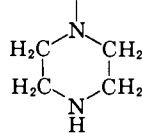
2.11.—The following trivial and semi-trivial names constitute a partial list of such names which are retained for the compound and as a basis of fusion names. They are arranged in the inverse order of the precedence prescribed in Rule B-3. The names of the radicals shown are formed according to Rule B-5.

	Parent Compound	Radical Name
(1)	 Thiophene	 Thieryl (2- shown)
(2)	 Benzo [<i>b</i>]thiophene (replacing thianaphthene)	 Benzo [<i>b</i>]thienyl (2- shown)
(3)	 Naphtho [2,3- <i>b</i>]thiophene (replacing thiophanthrene)	 Naphtho [2,3- <i>b</i>]thienyl (2- shown)

	Parent Compound	Radical Name
(4)	 Thianthrene	 Thianthrenyl (2- shown)
(5)	 Furan	 Furyl (3- shown)
(6)	 Pyran (2 <i>H</i> - shown)	 Pyranyl (2 <i>H</i> -Pyran-3-yl shown)
(7)	 Isobenzofuran	 Isobenzofuranyl (1- shown)
(8)	 Chromene (2 <i>H</i> - shown)	 Chromenyl (2 <i>H</i> -Chromen-3-yl shown)
(9)	 Xanthene ¹	 Xanthenyl ¹ (2- shown)
(10)	 Phenoxathiin	 Phenoxathiinyl (2- shown)
(11)	 2 <i>H</i> -Pyrrole	 2 <i>H</i> -Pyrrolyl (2 <i>H</i> -Pyrrol-3-yl shown)
(12)	 Pyrrole	 Pyrrolyl (3- shown)
(13)	 Imidazole	 Imidazolyl (2- shown)
(14)	 Pyrazole	 Pyrazolyl (1- shown)
(15)	 Pyridine	 Pyridyl (3- shown)
(16)	 Pyrazine	 Pyrazinyl

(1) Denotes exceptions to systematic numbering.

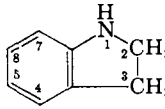
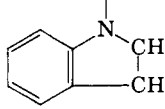
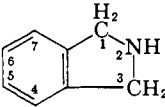
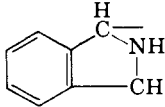
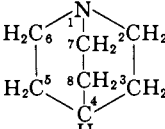
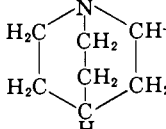
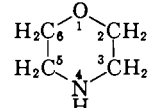
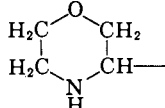
Parent Compound	Radical Name	Parent Compound	Radical Name
(17)  Pyrimidine	 Pyrimidinyl (2- shown)	(29)  Naphthyridine (1,8- shown)	 Naphthyridinyl (1,8-Naphthyridin-2-yl shown)
(18)  Pyridazine	 Pyridazinyl (3- shown)	(30)  Quinoxaline	 Quinoxaliny (2- shown)
(19)  Indolizine	 Indoliziny (2- shown)	(31)  Quinazoline	 Quinazoliny (2- shown)
(20)  Isoindole	 Isoindoly (2- shown)	(32)  Cinnoline	 Cinnoliny (3- shown)
(21)  3H-Indole	 3H-Indoly (3H-Indol-2-yl shown)	(33)  Pteridine	 Pteridinyl (2- shown)
(22)  Indole	 Indoly (1- shown)	(34)  4aH-Carbazole ¹	 4aH-Carbazoly ¹ (4aH-Carbazol-2-yl shown)
(23)  1H-Indazole	 Indazolyl (1H-Indazol-3-yl shown)	(35)  Carbazole ¹	 Carbazoly ¹ (2- shown)
(24)  Purine ¹	 Puriny ¹ (8- shown)	(36)  β -Carboline	 β -Carboliny (β -Carbolin-3-yl shown)
(25)  4H-Quinolizine	 4H-Quinoliziny (4H-Quinolizin-2-yl shown)	(37)  Phenanthridine	 Phenanthridinyl (3- shown)
(26)  Isoquinoline	 Isoquinoly (3- shown)	(38)  Acridine ¹	 Acridinyl ¹ (2- shown)
(27)  Quinoline	 Quinoly (2- shown)	(39)  Perimidine	 Perimidiny (2- shown)
(28)  Phthalazine	 Phthalazinyl (1- shown)		

	Parent Compound	Radical Name		Parent Compound	Radical Name
(40)	 Phenanthroline (1,7- shown)	 Phenanthrolyl (1,7-Phenanthrolin-3-yl shown)	(2)	 Chroman	 Chromanyl (7- shown)
(41)	 Phenazine	 Phenazinyl (1- shown)	(3)	 Pyrrolidine	 Pyrrolidiny (2- shown)
(42)	 Phenarsazine	 Phenarsaziny (2- shown)	(4)	 Pyrroline (2- shown ¹)	 Pyrroliny (2-Pyrrolin-3-yl ¹ shown)
(43)	 Isothiazole	 Isothiazoly (3- shown)	(5)	 Imidazolidine	 Imidazolidiny (2- shown)
(44)	 Phenothiazine	 Phenothiaziny (2- shown)	(6)	 Imidazoline (2- shown ¹)	 Imidazoliny (2-Imidazolin-4-yl ¹ shown)
(45)	 Isoxazole	 Isoxazoly (3- shown)	(7)	 Pyrazolidine	 Pyrazolidiny (1- shown)
(46)	 Furazan	 Furazany (3- shown)	(8)	 Pyrazoline (3- shown ²)	 Pyrazoliny (3-Pyrazolin-2-yl ² shown)
(47)	 Phenoxazine	 Phenoxaziny (2- shown)	(9)	 Piperidine	 Piperidyl ³ (2- shown)
(1)	 Isochroman	 Isochromanyl (3- shown)	(10)	 Piperazine	 Piperaziny (1- shown)

◆ *Chemical Abstracts* uses 2*H*-1-benzopyran instead of chromene, and 9*H*-pyrido[3,4-*b*]indole instead of β -carboline.

B-2.12.—The following trivial and semi-trivial names are retained but are not recommended for use in fusion names. The names of the radicals shown are formed according to Rule B-5.

- (1) The "2-" denotes the position of the double bond.
 (2) The "3-" denotes the position of the double bond.
 (3) For 1-piperidyl use piperidino.

Patent Compound	Radical Name
(11) 	
Indoline	Indolinyl (1- shown)
(12) 	
Isoindoline	Isoindolinyl (1- shown)
(13) 	
Quinuclidine	Quinuclidinyl (2- shown)
(14) 	
Morpholine	Morpholinyl ¹ (3- shown)

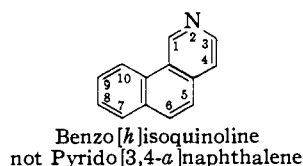
(1) For 4-morpholinyl use morpholino.

B-3. Fused Heterocyclic Systems

3.1.—“Ortho-fused” and “ortho- and peri-fused” ring compounds containing hetero atoms are named according to the fusion principle described in Rule A-21 for hydrocarbons. The components are named according to Rules A-21, B-1 and B-2. The base component should be a heterocycle. If there is a choice, the base component should be, by order of preference:

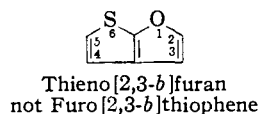
(a) A nitrogen-containing component.

Example:



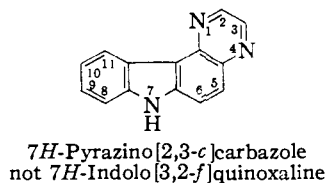
(b) A component containing a hetero atom (other than nitrogen) as high as possible in Table I.

Example:



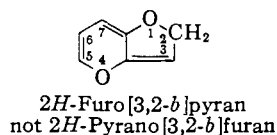
(c) A component containing the greatest number of rings.

Example:



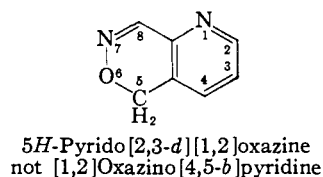
(d) A component containing the largest possible individual ring.

Example:



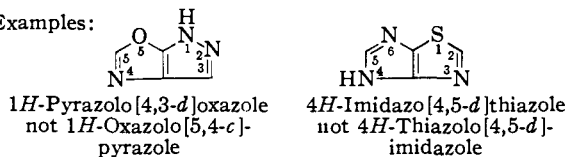
(e) A component containing the greatest number of hetero atoms of any kind.

Example:



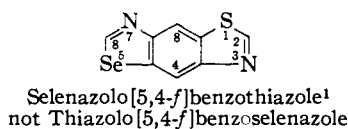
(f) A component containing the greatest variety of hetero atoms.

Examples:



(g) A component containing the greatest number of hetero atoms first listed in Table I.

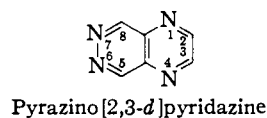
Example:



(1) In this example the hetero atom first listed in Table I is sulfur and the greatest number of sulfur atoms in a ring is one.

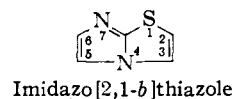
(h) If there is a choice between components of the same size containing the same number and kind of hetero atoms choose as the base component that one with the lower numbers for the hetero atoms before fusion.

Example:



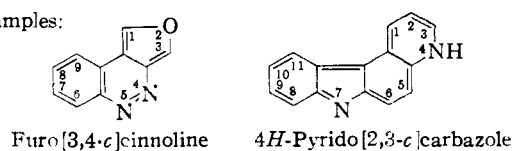
3.2.—If a position of fusion is occupied by a hetero atom, the names of the component rings to be fused are so chosen as both to contain the hetero atom.

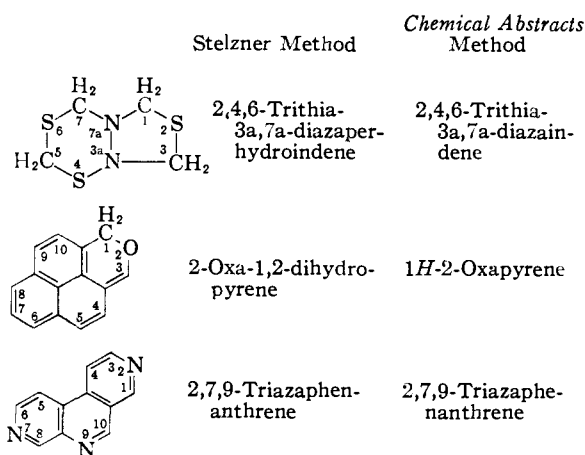
Example:



3.3.—These contracted fusion prefixes may be used: furo, imidazo, isoquino, pyrido, pyrimido, quino and thieno.

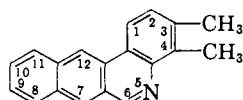
Examples:





4.2.—In fusion names, the “a” terms precede the completed name of the parent hydrocarbon. If two or more kinds of “a” terms occur in the same name, the procedure described in Rule B-1.4 applies. Prefixes denoting ordinary substitution precede the “a” terms.

Example:



3,4-Dimethyl-5-azabenz [a] anthracene

◆ *Chemical Abstracts* follows Rule B-4.1 (b). Since “a” names for heterocyclic systems are based on the name of the carbocyclic system, the numbering of the “a” name must agree with the numbering of the carbocyclic parent. When there is a choice in direction of numbering the ring is numbered so as to give (1) lowest numbers to the hetero atoms, (2) lowest numbers to hetero atoms as high as possible in Table 1 (Rule B-1.1).

B-5. Radicals

5.11.—Univalent radicals derived from heterocyclic compounds by removal of hydrogen from a ring are in principle named by adding “yl” to the names of the parent compounds (with elision of final “e” if present).

Examples: Indolyl from indole
Pyrrolinyl from pyrroline
Triazolyl from triazole
Triazinyl from triazine

(For further examples see Rule B-2.11.)

These exceptions are retained: furyl, pyridyl, piperidyl, quinolyl, isoquinolyl and thienyl (from thiophene) (see also Rule B-2.12).

As exceptions, the names “piperidino” and “morpholino” are preferred to “1-piperidyl” and “4-morpholinyl.”

5.12.—Bivalent radicals derived from univalent heterocyclic radicals whose names end in “-yl” by removal of one hydrogen atom from the atom with the free valence are named by adding “-idene” to the name of the corresponding univalent radical.

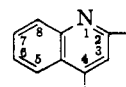
Example:



2-Pyranylidene

5.13.—Multivalent radicals derived from heterocyclic compounds by removal of two or more hydrogen atoms from different atoms in the ring are named by adding “-diyl,” “-triyl,” *etc.*, to the name of the ring system.

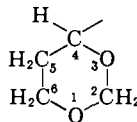
Example:



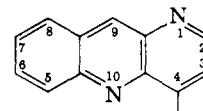
2,4-Quinolinediyl

5.21.—The use of “a” terms (Rule B-4) does not affect the formation of radical names. Such names are strictly analogous to those of the hydrocarbon analogs except that the “a” terms establish numbering in whole or in part.

Examples:



1,3-Dioxo-4-cyclohexyl

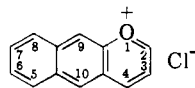


1,10-Diaza-4-anthryl

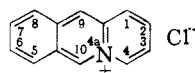
B-6. Cationic Hetero Atoms

6.1.—According to the “a” nomenclature, heterocyclic compounds containing cationic hetero atoms are named in conformity with the preceding rules by replacing “oxa-,” “thia-,” “aza-,” *etc.*, by “oxonia-,” “thionia-,” “azonia-,” *etc.*, the anion being designated in the usual way.

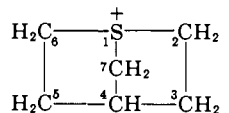
Examples:



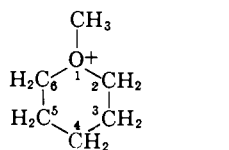
1-Oxonianthracene chloride



4a-Azonianthracene chloride



1-Thioniabicyclo[2.2.1]heptane chloride



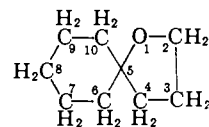
1-Methyl-1-oxoniacyclohexane chloride

HETEROCYCLIC SPIRO COMPOUNDS

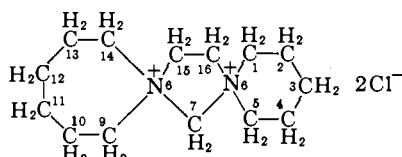
B-10 (Alternate to B-11)

10.1.—Heterocyclic spiro compounds containing single-ring units only may be named by prefixing “a” terms (see Table I, Rule B-1.1) to the names of the spiro hydrocarbons formed according to Rules A-41.1, A-41.2, A-41.3 and A-41.6. The numbering of the spiro hydrocarbon is retained and the hetero atoms in the order of Table I are given as low numbers as are consistent with the fixed numbering of the ring. When there is a choice, hetero atoms are given lower numbers than double bonds.

Examples:



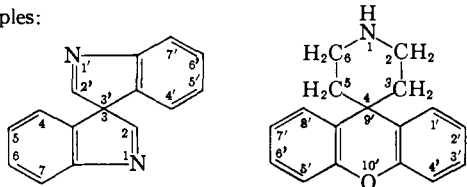
1-Oxaspiro[4.5]decane



6,8-Diazoniadispiro[5.1.6.2]hexadecane dichloride

10.2.—If at least one component of a mono- or polyspiro compound is a fused polycyclic system, the spiro compound is named according to Rule A-41.4 or A-41.7, giving the spiro atom as low a number as possible consistent with the fixed numberings of the component systems.

Examples:

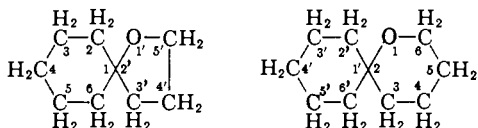
3,3'-Spirobi[3*H*-indole] Spiro[piperidine-4,9'-xanthene]

◆ *Chemical Abstracts* names heterocyclic spiro compounds according to Rules B-10.1 and B-10.2.

B-11 (Alternate to B-10)

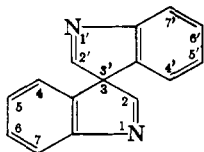
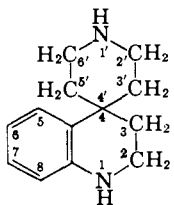
11.1.—Heterocyclic spiro compounds are named according to Rule A-42, the following criteria being applied where necessary: (a) spiro atoms have numbers as low as consistent with the numbering of the individual component systems; (b) heterocyclic components have priority over homocyclic components of the same size; (c) priority of heterocyclic components is decided according to Rule B-3. Parentheses are used where necessary for clarity in complex expressions.

Examples:

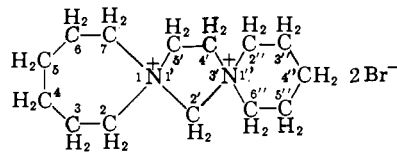


Cyclohexanespiro-2'-(tetrahydrofuran)

Tetrahydropyran-2'-spirocyclohexane

3,3'-Spirobi(3*H*-indole)

1,2,3,4-Tetrahydroquinoline-4-spiro-4'-piperidine



Hexahydroazepinium-1-spiro-1'-imidazolidine-3'-spiro-1''-piperidinium dibromide

◆ *Chemical Abstracts* follows Rule B-10.

BRIDGED HETEROCYCLIC COMPOUNDS

◆ Bridged heterocyclic bicyclo and polycyclo compounds are named by *Chemical Abstracts* by application of the "a" nomenclature to the names of bicyclo and polycyclo hydrocarbon systems which have been named according to Rules A-31 and A-32.

Bridged heterocyclic compounds which can be regarded as ortho-fused or ortho- and peri-fused systems with additional bridges are named by extending Rule A-34 to heterocyclic systems. Bridge names such as epoxy (—O—), epithio (—S—), epoxymethano (—O—CH₂—) are used.

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