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

NOMENCLATURE OF FUSED AND BRIDGED FUSED RING SYSTEMS

(IUPAC Recommendations 1998)

Prepared for publication by

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Names of countries given after members names are in accord with the *IUPAC Handbook 1996–1997.*

Nomenclature of fused and bridged fused ring systems (IUPAC Recommendations 1998)

Synopsis. These recommendations constitute a comprehensive documentation for naming fused ring systems and bridged fused ring systems. It expands and extends the recommendations given in rules A-21, A-22, A-23, A-34, B-3 of the *IUPAC Nomenclature of Organic Chemistry, Sections A, B, C, D, E, E, F and H*, 1979 and rule R-2.4.1 of *A Guide to IUPAC Nomenclature of Organic Compounds*, 1993. Any ring system with two or more rings *ortho-* or *ortho-* and *peri-*fused together may be named by these recommendations. Two rings which are *ortho*-fused together have only two atoms and one bond in common. The nomenclature of spiro systems and von Baeyer nomenclature will be considered in separate recommendations.

Contents

FR-0. Introduction

The general principles for naming polycyclic fused ring systems were proposed by Patterson (ref 1). These proposals were developed by a joint committee of the American Chemical Society and National Research Council and were approved by the IUPAC Committee on Organic Nomenclature before publication (ref 2). When sections A and B of the Nomenclature of Organic Chemistry (ref 3) were prepared this technique for naming polycyclic fused ring systems was adopted.

Chemical Abstracts Service (*CAS*) has developed this method to cover the more complex examples encountered in its work. These extensions were documented in the Ring Index (ref 2, 4) and in Chemical Abstracts (ref 5) while additions to the *Ring Index* were listed at first in just *Chemical Abstracts* (ref 6) and then in the *Parent Compound Handbook* (ref 7); they are now listed in the *Ring Systems Handbook* (ref 8). Some long established names used by *CAS* are retained by them although they would not be so named today. *Beilstein* too has had to extend and develop fusion nomenclature.

This document has been prepared from the sources mentioned above, and material from the Chemical Abstracts Service Substance Name Selection Manual. Assistance by *CAS* staff members is gratefully acknowledged.

Differences between the recommendations in this document and current *CAS* or *Beilstein* practice are indicated where appropriate.

Basic techniques for naming polycyclic fused ring systems are considered in a number of places in the 1979 IUPAC rules (ref 3). For hydrocarbons rules A-21, A-22, and A-23 cover the fused ring parent hydrides, which may then be used for the names of bridged systems (A-34). Heterocyclic examples are named using the extended Hantzsch-Widman system (ref 9) and selected trivial names (B-2.11 and Table IV in the appendix of Section D of ref 3, see also ref 3a, R-2.4.1) for heterocyclic components. Details of the fusion procedure are given in rule A-21.5 and B-3 (See also ref 3a, R-2.4.1). Replacement nomenclature is described in rules B-4, B-6 and D-1.6 (See also ref 3a, R-1.2.2 and R-2.3.3.2).

This document provides a unified treatment of heterocyclic and hydrocarbon polycyclic fused ring systems with recommendations for the naming of complex examples not covered by the 1979 IUPAC rules. All names are for fused ring systems with the maximum number of non-cumulative double bonds even though the system may only be known in the form of a partially or fully hydrogenated derivative.

Structures in this document are drawn as far as possible with undistorted rings. It should be noted that the use of distorted ring shapes is only necessary for the orientation of ring systems prior to numbering the system (FR-5).

In this document no restriction is placed on when fusion nomenclature may be applied. Previously (rule A-21.3 of ref 3) it was restricted to systems which contain at least two rings of five or more members.

FR-1. Definitions

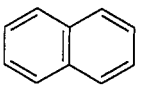
FR-1.1 Fusion

Fusion nomenclature is concerned with a two dimensional representation of a polycyclic ring system with the maximum number of non-cumulative double bonds. In addition this system may be bridged (see FR-8), or involved in assemblies or spiro systems (not covered by these rules). For ring systems any ring fused to other rings on all sides must be itself named (*i.e.* it is not treated as a hole). For nomenclature purposes two rings which have two atoms and one bond in common may be regarded as being derived from the two rings as separate entities. The process of joining rings in this way is termed fusion.

FR-1.1.1 *Ortho-fused*

Two rings that have only two atoms and one bond in common are said to be *ortho*-fused.

Example:

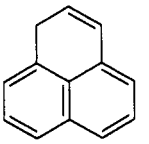


The two benzene rings of naphthalene are *ortho*-fused together

FR-1.1.2 *Ortho- and peri-fused*

In a polycyclic compound, a ring *ortho*-fused to different sides of two other rings that are themselves *ortho*-fused together (i.e. there are three common atoms between the first ring and the other two) is said to be *ortho*- and *peri*-fused to the other two rings.

Example:



Phenalene is considered as being composed of three benzene rings, each of which is *ortho*- and *peri*-fused to the other two.

FR-1.1.3 *Fusion atom*

Any atom of a fused ring system which is common to two or more rings is termed a fusion atom.

FR-1.1.4 *Peripheral atom*

An atom that forms part of the outer perimeter of a fused ring system is called a peripheral atom.

FR-1.1.5 *Bridgehead atom*

An atom of a fused ring system to which a bridge (see FR-1.4) is attached is called a bridgehead atom.

FR-1.1.6 *Interior atom*

Any fusion atom which is not a peripheral atom is termed an interior atom.

FR-1.2 Fused ring system

A system where each bond is part of a ring; where each ring is *ortho*-fused (FR-1.1.1), or *ortho*- and *peri*-fused (FR-1.1.2), to at least one other ring; and where no bond is common to more than two rings is termed a fused ring system.

FR-1.2.1 *Bridged fused ring system*

A ring system where some of the rings constitute a fused ring system and the remaining rings are created by one or more bridges (FR-1.4) is termed a bridged fused ring system.

FR-1.2.2 *Multiparent name*

A fused ring system name which is constructed using an interparent component (FR-1.3.3) and two or more identical parent components (FR-1.3.1) is called a multiparent name.

FR-1.2.3 *Multiplicative prefix name*

A fused ring system name which is constructed using one or more multiplicative prefix(es) (di-, tri-, *etc.* or bis-, tris-, *etc.*) to indicate multiple occurrences of the attached component(s) (FR-1.3.2) is called a multiplicative prefix name.

FR-1.3 Components of a fused ring system

Allowed fusion components are rings or ring systems which can be named without the application of any fusion nomenclature principles (see Appendices 1 and 2). Fused ring systems which do not have such a name are named by joining together appropriately selected fusion components.

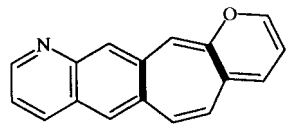
FR-1.3.1 *Parent component*

The parent component (referred to as the base or principle component in previous versions of these rules) is the one with highest seniority according to the criteria given in FR-2.3 and is represented in the fusion name by that ring or ring system which is cited last in the name. It may be mono- or poly-cyclic (see FR-1.3.2 for an example).

FR-1.3.2 *Attached component(s)*

The components of a fused ring system which are not covered by the parent component are called attached component(s) and are expressed by fusion prefixes. Prefixes denoting components directly fused to the parent component are called first-order fusion prefixes. The rest are called second-order, third-order, *etc.* fusion prefixes which means they correspond to the second, third, *etc.* component reached when moving away from the parent component across fusion sites. All attached components may be mono- or poly-cyclic.

Example:



Parent component - quinoline
First-order fusion prefix - cyclohepta
Second-order fusion prefix - pyrano

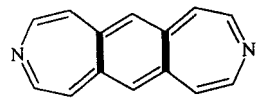
pyrano[2',3':4,5]cyclohepta[1,2-*g*]quinoline

Note Details of the method for naming fused ring systems are not given until FR-4.

FR-1.3.3 *Interparent component(s)*

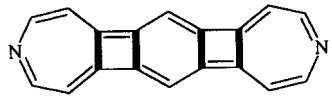
In a system that consists of two (or more) parent components *ortho-*, or *ortho-* and *peri*-fused to the same attached component the latter is called the first-order interparent component. Likewise if two (or more) parent components are linked by three appropriately attached components there will be two identical first-order interparent components and a second-order interparent component. Systems with five or more interparent components are regarded in a similar way (see FR-6 for the special rules used to name systems with interparent components).

Examples:



Parent component - azepine
Interparent component - benzo

benzo[1,2-*d*:4,5-*d*']bisazepine



Parent component - azepine
First-order interparent component - cyclobuta
Second-order interparent component - benzo

benzo[1",2":3,4;4",5":3',4']dicyclobuta[1,2-*d*:1',2'-*d*']bisazepine

FR-1.4 **Bridges**

An atom or group of atoms is named as a bridge by means of a prefix if it fulfils one or more of the following criteria:

a. If it connects two or more non-adjacent positions of the same ring in a fused ring system.

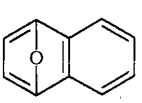
b. If it connects two or more positions of different rings of a fused ring system and does not thereby form a new *ortho-* and *peri*-fused ring.

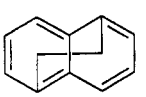
c. If it connects positions in a ring of a fused ring system to a previously described bridge but cannot be included as part of that bridge (an independent bridge: see FR-1.4.6).

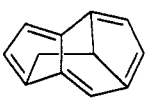
d. If it connects the atoms at the end of a bond common to two rings of a fused ring system.

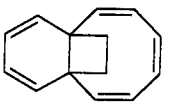
e. If it is necessary to describe a system with only *ortho-* or *ortho-* and *peri*-fusions but which cannot be completely named by fusion principles (see FR-7).

Examples:


criterion a


criterion b

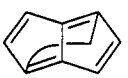
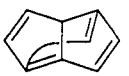

criterion b


criterion d

Notes 1. See rule A-31.1 (ref 3) for a different definition of a bridge in a von Baeyer system.

2. *Beilstein* uses cyclo to indicate a direct bond between two non-adjacent positions of a fused ring system [*cf.* rule F-4.1 (ref 3) for use with natural products]. For example, the skeleton below (see also note 3) is named by *Beilstein* as 1,5-cycloindene instead of as a bridged pentalene. The preferred bridged pentalene has a bivalent bridge (see FR-8.2.h).

   Example:


not

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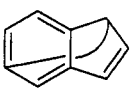


   With complex systems cyclo may facilitate generation of names. For example FR-8.2.i is illustrated by a system which could be called 3,4-cyclo-2,5-(metheno)dipentaleno-[2,1-*f*:2',1'-*f*']cyclopenta[2,1-*a*:3,4-*a*']dipentalene (see FR-5.4.c for numbering)

3. For the purposes of naming polycyclic fused and bridged fused ring systems the parent hydride is considered as a two-dimensional skeleton with normally the maximum number of non-cumulative double bonds in the fused ring system [*i.e.* excluding the bridge(s)]. The exceptions to this situation are when there is a double bond between a bridge and a fused ring system in the structure under consideration (*i.e.* requiring the use of the ending '-ylidene', see FR-8.3.2), or when a bridge terminates at an existing fusion atom or a trivalent atom, (see FR-8.1.2). In considering alternative ways of naming a bridged fused ring system the number and location of the double bonds in alternative parent structures may vary. Also the parent structure so described may not exist as such, but only in a hydrogenated or partially hydrogenated form. For example although all three structures in note 2 above have the same skeleton the double bonds of the preferred structure are located differently from the other two, since the maximum number of non-cumulative double bonds is always assigned in the *ortho*- or *ortho*- and *peri*-fused portion (see FR-9.1).

FR-1.4.1 *Simple bridge prefix*

A simple bridging prefix describes an atom, or group of atoms that may be considered as a single unit *e.g.* epoxy, butano, benzeno.

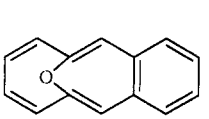
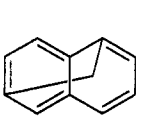
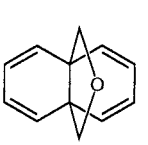
FR-1.4.2 *Composite bridge prefix*

A composite bridge prefix describes a group of atoms that can only be considered as a contiguous sequence of simple bridges *e.g.* (epoxymethano) = epoxy + methano = $-O-CH_2-$. It has also been called a compound bridge prefix.

FR-1.4.3 *Bivalent bridge*

A bivalent bridge is one which is connected by single bonds to two different positions of a fused ring system or a bridged fused ring system.

Examples:

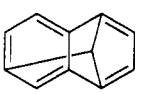




FR-1.4.4 *Polyvalent bridge*

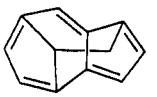
A polyvalent bridge is one that is connected to a fused ring system by three or more single bonds or their multiple bond equivalents. A polyvalent bridge may often be considered as a combination of two bivalent simple bridges - one first-order and the other dependent.

Polyvalent bridges may be further classified as bipodal, tripodal *etc.* where the bridge is attached at two positions, three positions *etc.*

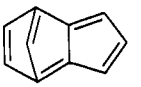
Examples:



tripodal bridge



tripodal bridge



bipodal bridge

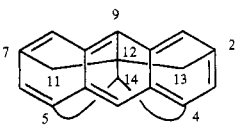
FR-1.4.5 *Independent bridge*

A bridge which only connects two or more positions of a fused ring system is called an indepenent bridge. See example with FR-1.4.6.

FR-1.4.6 *Dependent bridge*

A bridge which connects one or more positions of a fused ring system to one or more positions on a simple or composite independent bridge, and cannot be expressed as part of a larger composite bridge is called a dependent bridge.

Example:



4,5,12-(methanetriyl)-2,9,7-(propane[1,2,3]triyl)anthracene
the methanetriyl group C-14 is a dependent bridge
the propane[1,2,3]triyl group at C-11 to C-13 is an independent bridge

FR-2 Ring Systems Used as Components

The names of polycyclic fused ring systems are derived from those of components which are themselves mono- or poly-cyclic ring systems.

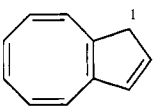
FR-2.1 Hydrocarbon components

Hydrocarbon parent components are listed in Appendix 1. The components are listed in decreasing order of preference for choice of components (see FR-2.3).

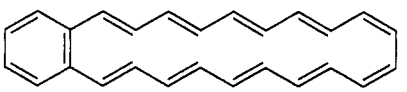
FR-2.1.1 *Monocyclic hydrocarbon components*

Monocyclic hydrocarbon parent components (other than benzene) are named as [*n*]annulenes, where *n* represents the ring size. The corresponding attached component prefix is derived from the appropriate cycloalkane stem with the ending '-a'.

Examples:



1*H*-cyclopenta[8]annulene
CAS and *Beilstein* name 1*H*-cyclopentacyclooctene



benzo[22]annulene
CAS and *Beilstein* name benzocyclodocosene

Notes 1. In previous versions of these rules (ref 3, A-21.4)) the parent component was named from the cycloalkane stem with the ending '-ene'. This would normally imply one double bond in the ring in contrast to the meaning here of the system with the maximum number of non-cumulative double bonds. Use of the [*n*]annulene terminology prevents any confusion. The traditional names of the attached components are retained.

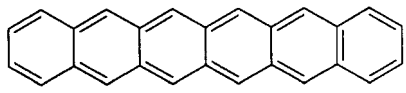
2. [*n*]Annuleno is not used as a prefix.

3. The alternative method for the naming of these systems described in rule A-23.5 (ref 3) is abandoned.
4. [*n*]Annulene with $n < 6$ is only used as a parent component not for the isolated system.

FR-2.1.2 *Polyacene components*

A hydrocarbon parent component that consists of four or more *ortho*-fused benzene rings in a straight linear arrangement is named from the numerical prefix (ref 10) denoting the number of benzene rings followed by the ending '-acene' (derived from anthracene). In an attached component prefix the ending '-acene' is changed to '-aceno'. Note that tetracene was called naphthacene in rule A-21.1 (ref 3) and this is still used by *CAS* and *Beilstein*.

Example:

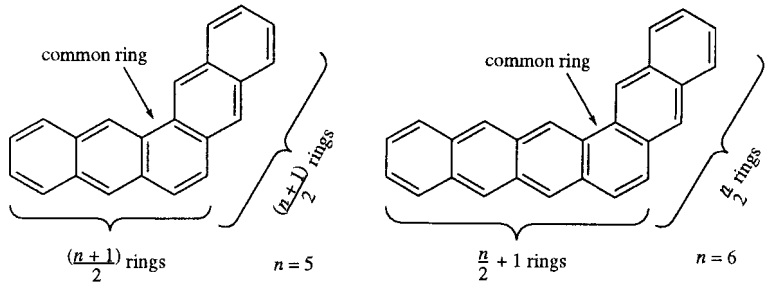


pentacene

FR-2.1.3 *Polyaphene components*

A hydrocarbon parent component that consists of *n ortho*-fused benzene rings ($n > 3$) and comprises two straight linear arrangements of $(n+1)/2$ and $(n+1)/2$ (if *n* is odd) or $n/2$ and $(n/2)+1$ rings (if *n* is even) with a common benzene ring and which make a formal angle of 120° is named by citing the numerical prefix (ref 10) denoting the total number of benzene rings followed by the ending '-aphene' (derived from **phen**anthrene). In an attached component prefix the ending '-aphene' is changed to '-apheno'.

Examples:

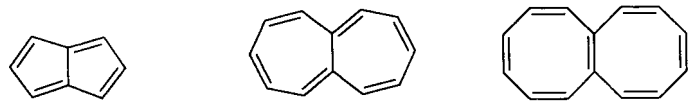


pentaphene hexaphene

FR-2.1.4 *Polyalene components*

A hydrocarbon parent component that consists of two identical *ortho*-fused monocyclic hydrocarbon rings is named from the numerical prefix (ref 10) denoting the number of carbon atoms in each ring and the ending '-alene'. The trivial name naphthalene is retained for hexalene. In an attached component prefix the ending '-alene' is changed to '-aleno'.

Examples:



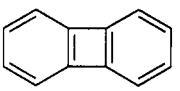
pentalene heptalene octalene

FR-2.1.5 *Polyphenylene components*

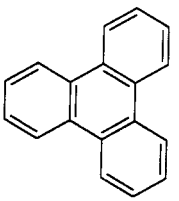
A hydrocarbon parent component that consists of a monocyclic hydrocarbon with an even number of carbon atoms and benzene rings *ortho*-fused to alternate sides is named from the numerical prefix (ref 10) denoting the number of benzene rings followed by the ending '-phenylene'. In an attached component prefix the

ending '-phenylene' is changed to '-phenyleno'. As an exception the first member of the series is called biphenylene instead of diphenylene.

Examples:



biphenylene

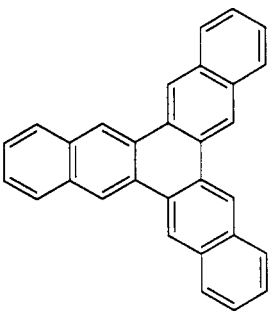


triphenylene

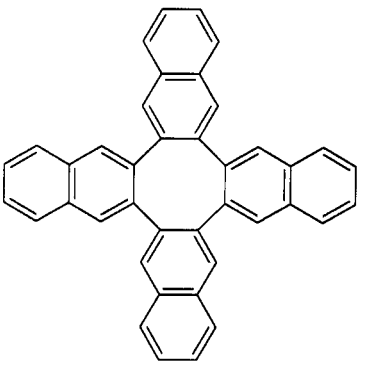
FR-2.1.6 *Polynaphthylene components*

A hydrocarbon parent component that consists of a monocyclic hydrocarbon with an even number of carbon atoms and with naphthalene ring systems 2,3-fused to alternate sides is named from the numerical prefix (ref 10) denoting the number of naphthalene units followed by the ending 'naphthylene'. In an attached component prefix the terminal '-e' is changed to '-o'. The first member of the series (with two naphthalene ring systems) is called dibenzo[*b*,*h*]biphenylene and is not used as a component.

Examples:



trinaphthylene

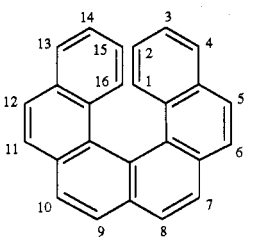


tetranaphthylene

FR-2.1.7 *Polyhelicene components*

A hydrocarbon parent component of six or more rings that consists of a benzene ring fused to the 3,4-position of phenanthrene and further benzene rings fused in a similar way is named from the numerical prefix (ref 10) denoting the total number of rings followed by the ending '-helicene'.

Example:



hexahelicene

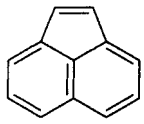
CAS and *Beilstein* name phenanthro[3,4-*c*]phenanthrene

The numbering of these ring systems using FR-5 presents a problem due to ring overlap and that the ring where numbering should start depends on the number of rings present. To circumvent this problem it is recommended that a terminal ring be numbered from 1 to 4 followed in the normal way round the external peripheral atoms followed by the internal peripheral atoms. See 32 in Appendix 1.

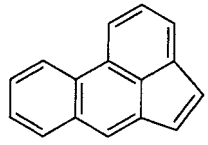
Note Polyhelicene names are not used in *CAS* index nomenclature.

FR-2.1.8 *Ace ....ylene components*

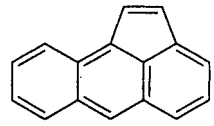
A hydrocarbon parent component that consists of a five-membered ring *ortho-* and *peri*-fused to naphthalene, anthracene or phenanthrene is named by adding the prefix 'ace-' and changing the ending '-alene', '-acene' or '-ene', respectively to '-ylene'.



acenaphthylene



acephenanthrylene



aceanthrylene

FR-2.1.9 *Trivially named hydrocarbon components*

The trivially named hydrocarbons used as parent components in fusion nomenclature are listed below. The reference numbers refer to the entry in Appendix 1.

anthracene	47	(see FR-2.1.2 for other straight linear systems)	naphthalene	57	
azulene	56		ovalene	10	
benzene	62	(see FR-2.1.1 for other monocycles)	perylene	36	
chrysene	41		phenalene	49	
coronene	26		phenanthrene	48	(see FR-2.1.3 for other bent linear systems)
fluoranthene	46		picene	37	
fluorene	50		pleiadene	38	
as-indacene	54		pyranthrene	20	
s-indacene	53		pyrene	42	
indene	58		rubicene	28	

In an attached component prefix the ending '-ene' is changed to '-eno', *e.g.* pyreno (from pyrene). Only the following abbreviated forms are used:

anthra from anthracene	naphtho from naphthalene
benzo from benzene	phenanthro from phenanthrene

Notes 1. Rule A-21.4 (ref 3) also recommended the abbreviation of acenaphthyleno and peryleno to acenaphtho and perylo, which are still used by *CAS* and *Beilstein*.

2. The non-standard numberings of anthracene and phenanthrene are retained (see Appendix 1).

3. *CAS* and *Beilstein* also include trindene (cyclopenta[*e*]-*as*-indacene).

FR-2.2 **Heterocyclic component**

Heterocyclic parent components are listed in Appendix 2. The components are listed in decreasing order of preference (see FR-2.3).

FR-2.2.1 *Heteromonocyclic components*

a. The following trivial names are retained for heteromonocyclic parent components. The reference numbers refer to the entry in Appendix 2.

furan	71	pyridazine	48	selenophene	83
imidazole	53	pyridine	49	tellurophene	88
pyran	69	pyrimidine	47	thiophene	78
pyrazine	48	pyrrole	54	thiopyran	78
pyrazole	52				

In an attached component prefix the terminal 'e' is changed to 'o' (or the 'o' is added in the case of pyran and chalcogen analogues). Only the following abbreviated forms are used:

furo from furan	pyrimido from pyrimidine
imidazo from imidazole	thieno from thiophene
pyrido from pyridine	

These abbreviated forms are also used in combined forms *e.g.* benzofuro (see FR-2.2.8).

Note 1. In the previous edition of these rules oxazole, isoxazole, thiazole and isothiazole were used as component names. When combined in heterobicyclic names with a benzene ring (FR-2.2.8) locants were required for the iso case. The full Hantzsch-Widman name is now recommended for fusion names *i.e.* 1,3-oxazole, 1,2-oxazole, 1,3-thiazole and 1,2-thiazole respectively. The traditional names are retained in these recommendations for use with the isolated ring system and are still used as fusion components by *CAS* and *Beilstein* together with selenazole, isoselenazole, tellurazole and isotellurazole.

2. *Beilstein* uses selenopyran and telluropyran instead of selenine and tellurine.

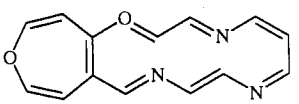
b. A heteromonocyclic parent component with a ring of up to ten members not listed in FR-2.2.1(a) is named using the extended Hantzsch-Widman system (ref 9). In an attached component prefix the terminal 'e' is changed to 'o'. In fused ring names where locants are needed to locate the heteroatoms in a component ring these locants are cited in square brackets (see FR-4.8).

Notes 1. In the Hantzsch-Widman system (ref 9) the terminal 'e' is optional. In this document the 'e' is included. If the 'e' is omitted the terminal '-in' is changed to '-ino'.

2. The Hantzsch-Widman suffix is that appropriate for a mancude (maximum number of non-cumulative double bonds) ring system.

c. A heteromonocyclic parent component with more than ten members is named by modifying the corresponding heterocycloalkane name changing the ending '-ane' to '-ine'. In an attached component prefix the terminal 'e' is changed to 'o'. If locants are needed to locate the heteroatoms these are cited in square brackets (see FR-4.8). Where there is a choice of locants they are selected as in the Hantzsch-Widman system.

Example:



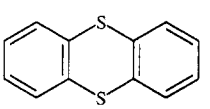
oxepino[4,5-*m*][1,4,8,11]oxatriazacyclotetradecine

Note When a heteromonocyclic component with more than ten members is present *Beilstein* uses replacement nomenclature. Thus the example above is called 3,6-dioxa-9,13,16-triaza-cycloheptacyclotetradecene by *Beilstein.*

FR-2.2.2 *Heteranthrene components*

A heterotricyclic parent component that consists of two benzene rings fused to a 1,4-diheterabenzene in which the heteroatoms are the same is named from the appropriate replacement prefix (Table 1 of RB-1.1 in ref 9) and the suffix '-anthrene' with elision of the 'a'.

Example:



thianthrene

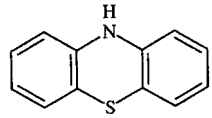
In an attached component prefix the ending '-ene' is changed to '-eno'.

Appendix 2 includes this system for O, S, Se, Te, P, As, Si, B, and Hg (entries 63, 74, 79, 84, 89, 99, 109, 110, and 111 in appendix 2). The nitrogen analogue is an exception and is named phenazine. Boranthrene, oxanthrene, silanthrene and telluranthrene were not included previously (ref 3). Oxanthrene is still called dibenzo[1,4]dioxin by *CAS* and *Beilstein.* Mercuranthrene, formerly called phenomercurin (ref 3) or phenomercurine (ref 3a), is called *cyclo*-di-μ-1,2-phenylenedimercury by *CAS.*

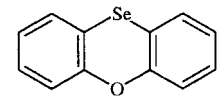
FR-2.2.3 *Pheno....ine components*

A heterotricyclic parent component that consists of two benzene rings fused to a 1,4-diheterabenzene in which the heteroatoms are different is named by adding the prefix 'pheno-' to the Hantzsch-Widman name (ref 9).

Examples:



10*H*-phenothiazine



phenoxaselenine

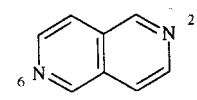
In an attached component prefix the ending '-ine' is changed to '-ino' (see note 1 to FR-2.2.1.b).

Appendix 2 includes this system for NH with O, S, Se and Te (entries 1-4); N with P, As and Hg (with the reverse order of 'a'-prefixes for entries 5-7); O with S, Se, Te, PH, AsH and SbH (entries 57-62); and S with AsH (entry 73). Phenoxastibinine was previously called phenoxantimonine. 2*H*-Phenomercurazine, formerly called 2*H*-phenomercazine, is called (3,6-cyclohexadien-1-yl-2-ylidenenitrilo-1,2-phenylene)mercury by *CAS*.

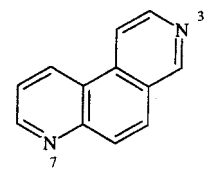
FR-2.2.4 *Diazanaphthalene and diazaphenanthrene components*

A heterocyclic component which corresponds to naphthalene or phenanthrene where each terminal ring has one non-fusion atom replaced by nitrogen is called naphthyridine or phenanthroline respectively. The location of the two nitrogen atoms is indicated by the appropriate locants [see Appendix 2 for the range of isomers possible for naphthyridine (entries 27-30, 32 and 33) and phenanthroline (entries 9-18)].

Examples:



2,6-naphthyridine



3,7-phenanthroline

Note Phenanthroline is numbered in the standard way (see FR-5.3) despite the non-standard numbering of phenanthrene.

FR-2.2.5 *Trivially named polycyclic, nitrogen-heterocyclic components*

The following trivial names of nitrogen heterocycles are also used as parent components in fusion nomenclature. In an attached component prefix the terminal 'e' is changed to 'o' *e.g.* indolo (from indole). The reference numbers below refer to Appendix 2.

acridine	20	isoquinoline	35	pteridine	23
carbazole	22	naphthyridine	(see FR-2.2.4)	purine	37
cinnoline	24	perimidine	19	pyrrolizine	42
indazole	38	phenanthridine	21	quinazoline	25
indole	39	phenanthroline	(see FR-2.2.4)	quinoline	34
indolizine	41	phenazine	(see FR-2.2.2)	quinolizine	36
isoindole	40	phthalazine	31	quinoxaline	26

Notes 1. Rule B-3.3 (ref 3) recommended the abbreviation of isoquinolino to isoquino and quinolino to quino. These abbreviated forms are not used here but are still used by *CAS* and *Beilstein*.

2. β-Carboline (pyrido[3,4-*b*]indole) was abandoned as a component name in 1979 (ref 3).

3. Acrindoline, anthrazine, anthyridine, phenanthrazine, phthaloperine, quindoline, quinindoline, thebenidine, triphenodioxazine and triphenodithiazine are used as component names by *CAS* (see note a of appendix 2).

4. 1-Pyrindene (cyclopenta[*b*]pyridine) and 2-pyrindene (cyclopenta[*c*]pyridine) are used by *CAS* and *Beilstein* for the isolated ring system but not as a component for fusion.

FR-2.2.6 *Components formed by replacement of nitrogen by arsenic or phosphorus*

The following parent components containing arsenic or phosphorus are named by adaption of the corresponding nitrogenous parent component names. The reference number refers to the entry in Appendix 2.

Nitrogen		Arsenic		Phosphorus	
acridine	20	acridarsine	100	acridophosphine	90
indole	39	arsindole	105	phosphindole	95
indolizine	41	arsindolizine	107	phosphindolizine	97
isoindole	40	isoarsindole	106	isophosphindole	96
isoquinoline	35	isoarsinoline	103	isophosphinoline	93
phenanthridine	21	arsanthridine	101	phosphanthridine	91
quinoline	34	arsinoline	102	phosphinoline	92
quinolizine	36	arsinolizine	104	phosphinolizine	94

In an attached component prefix the terminal 'e' is changed to 'o'.

FR-2.2.7 *Trivially named polycyclic, chalcogen-heterocyclic components*

The following trivial names of chalcogen heterocycles are also used in fusion nomenclature. The reference number refers to Appendix 2.

Chromene	65	Isochromene	66	Xanthene	64
Thiochromene	76	Isothiochromene	77	Thioxanthene	75
Selenochromene	81	Isoselenochromene	82	Selenoxanthene	80
Tellurochromene	86	Isotellurochromene	87	Telluroxanthene	85

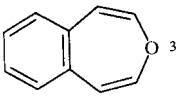
In an attached component prefix the terminal 'e' is changed to 'o', e.g. xantheno (from xanthene).

Note Chromene and isochromene and the chalcogen analogues are not used by *CAS* but are used by *Beilstein*. *CAS* uses 1-benzopyran, 2-benzopyran *etc.*

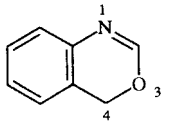
FR-2.2.8 *Heterobicyclic components with a benzene ring*

Unless listed as a trivially named heterobicycle in Appendix 2 a benzene ring fused to a heteromonocycle of five or more members (a benzoheterocycle) is named by prefixing number locants indicating the position(s) of the heteroatom(s) to benzo followed by the trivial, Hantzsch-Widman, or modified replacement name (see FR-2.2.1) of the heteromonocycle without locants. The locants quoted correspond to the numbering of the bicyclic structure, which follows FR-5.4. Locants are not needed if their omission does not result in ambiguity, *e.g.* benzimidazole, benzotriazole. As an exception to FR-4.7 the 'o' of benzo is elided if followed by a vowel. See FR-3.5 for the use of this type of name as a component and FR-4.8 for the use of square brackets around locants. Brackets are not used for the unmodified ring system.

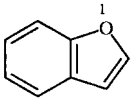
Examples:



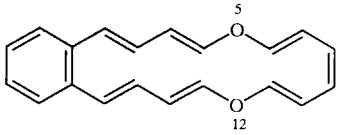
3-benzoxepine



4*H*-3,1-benzoxazine



1-benzofuran



5,12-benzodioxacyclooctadecine

Names of this type are only used as components under certain conditions; see FR-3.5 for the details. *Beilstein* does not use this type of name.

Notes 1. 1-Benzofuran and 2-benzofuran were formerly called benzofuran and isobenzofuran (ref 3) and may still be used for the isolated ring system. *CAS* still uses benzofuran and isobenzofuran as fusion components.

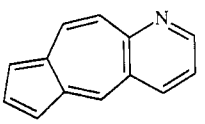
2. 1,2-Benzoxazole and its 2,1- and 1,3-isomers and chalogen analogues were called 1,2-benzisoxazole, 2,1-benzisoxazole, benzoxazole, *etc.* These are still used by *CAS* for the isolated ring system and as fusion components.

FR-2.3 Priority order of component ring systems

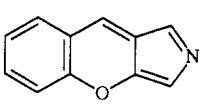
Selection of a parent component (see FR-3.3) or attached component (see FR-3.4) is based on the following rules which are applied in order. Appendices 1 and 2 list the hydrocarbon and heterocyclic components in decreasing order of preference. If there is a choice, the preferred component should be:

a. A heterocyclic component containing the heteroatom occurring earliest in the order N, F, Cl, Br, I, O, S, Se, Te, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Hg [see Table 1 of the revised Hantzsch-Widman system (ref 9) with the exception of nitrogen].

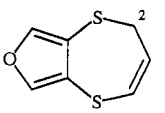
Examples:



azuleno[6,5-*b*]pyridine
(pyridine preferred to azulene)



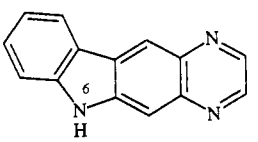
chromeno[2,3-*c*]pyrrole
(pyrrole preferred to chromene)



2*H*-[1,4]dithiepino[2,3-*c*]furan
(furan preferred to dithiepine)

b. A component containing the greater number of rings.

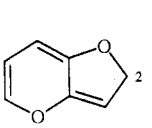
Example:



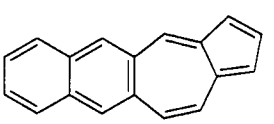
6*H*-pyrazino[2,3-*b*]carbazole
(carbazole [3 rings] preferred to quinoxaline [2 rings])

c. A component containing the larger ring at the first point of difference when comparing rings in order of decreasing size.

Examples:



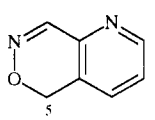
2*H*-furo[3,2-*b*]pyran
(pyran [6] preferred to furan [5])



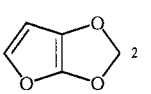
naphtho[2,3-*f*]azulene
(azulene [7,5] preferred to naphthalene [6,6])

d. A component containing the greater number of heteroatoms of any kind.

Examples:



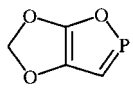
5*H*-pyrido[2,3-*d*][1,2]oxazine
(oxazine preferred to pyridine)



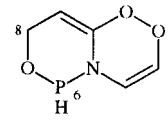
2*H*-furo[2,3-*d*][1,3]dioxole
(dioxole preferred to furan)

e. A component containing the greater variety of heteroatoms.

Examples:



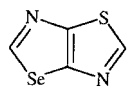
[1,3]dioxolo[*d*][1,2]oxaphosphole
(O and P preferred to only O)



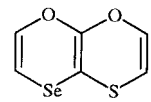
6*H*,8*H*-[1,2,4]dioxazino[4,3-*c*][1,3,2]oxazaphosphinine
(O, N and P preferred to O and N)

f. A component containing the greater number of heteroatoms most preferred when considered in the order F, Cl, Br, I, O, S, Se, Te, N, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Hg [*i.e.* Table I of the revised Hantzsch-Widman system (ref 9)].

Examples:



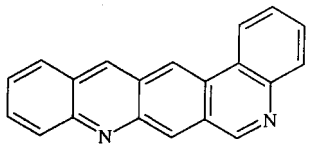
[1,3]selenazolo[5,4-*d*][1,3]thiazole
(S,N preferred to Se,N)



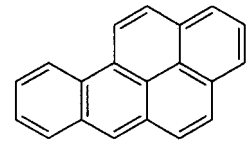
[1,4]oxaselenino[2,3-*b*][1,4]oxathiine
(O,S preferred to O,Se)

g. A component in the preferred orientation according to FR-5.2.

Examples:



quinolino[4,3-*b*]acridine
(acridine [3 rings in row] preferred to
phenanthridine [2 rings in row] FR-5.2.a)

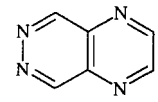


benzo[*pqr*]tetraphene
(tetraphene [3 rings in row] preferred to
chrysene or pyrene [2 rings in row] FR-5.2.a)

Note The second example is called benzo[*a*]pyrene by *CAS* as an exception to this rule.

h. A component with the lower locants for heteroatoms.

Example:

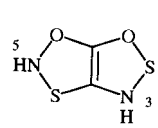


pyrazino[2,3-*d*]pyridazine
(pyridazine [1,2] preferred to pyrazine [1,4])

Note Quinolizine is an exception to this rule in *CAS* where it is preferred to quinoline or isoquinoline.

i. A component with the lower locants for the heteroatoms when considered in the order F, Cl, Br, I, O, S, Se, Te, N, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Hg [*i.e.* Table I of the revised Hantzsch-Widman system (ref 9)].

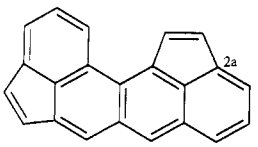
Example:



3*H*,5*H*-[1,3,2]oxathiazolo[4,5-*d*][1,2,3]oxathiazole
(1,2,3 preferred to 1,3,2)

j. A component with the lower locants for bridgehead carbon atoms.

Example:



indeno[1,7-*kl*]aceanthrylene
(aceanthrylene [2a] preferred to acephenanthrylene [3a])

FR-2.4 Natural products and fullerenes

Fusion of components to natural products and fullerenes are not included in this document. Details have been published for carbohydrates (ref 11), steroids (ref 12) and tetrapyrroles (ref 13) and there are proposals for prostaglandins, thromboxanes (ref 14), natural products in general (ref 15) and fullerenes (ref 16).

FR-3 Construction of Fusion Names

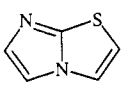
FR-3.1 *Ortho*-, or *ortho*- and *peri*-fused systems

Before naming a polycyclic parent hydride containing a fused ring system it is necessary to identify the bridges (if any) which are treated separately from the *ortho*- or *ortho*- and *peri*-fused system (see FR-8).

FR-3.2 Selection of components

Each ring and/or combination of rings in a fused ring system is considered in order to select the parent component(s) (see FR-3.3). The first-order attached component(s) is then selected (if necessary) followed by second-order attached component(s) and higher-order attached components (see FR-3.4). It should be noted that when a heteroatom is common to two components it must be indicated in the name of each component.

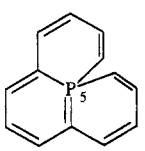
Example:



imidazo[2,1-*b*][1,3]thiazole

If an atom is in a non-standard valence state this is indicated using the λ-convention (ref 17). The bonding number *n* is cited as a superscript *i.e.* λ^n, together with the locant of the atom with a non-standard valence state, in front of the name of the fused ring system (see FR-9.1).

Example:



5λ^5-phosphinino[2,1-*d*]phosphinolizine

Note Fusion nomenclature provides no means of describing the fusion of one component to two other components which are themselves fused together. If this problem arises see FR-7 for examples and how to name them.

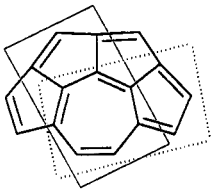
FR-3.3 Selection of parent component(s)

The ring or rings selected as the parent component are those most preferred by the criteria of FR-2.3 (see examples therein). The parent component may be identified in more than one location in a fused ring system by using different rings or combinations of rings. Such alternative locations of the parent component may be overlapping; or directly fused together; or separated by one or more components. When there are alternative locations for the parent component(s) the criteria of FR-3.3.1 are used to select the preferred location(s).

FR-3.3.1 *Order of preference between locations for parent components*

If there are two or more potential locations for a parent component the following criteria apply in order until a distinction is obtained. If a partial distinction is obtained the following criteria are only applied to distinguish between remaining choices. In the examples below the preferred location(s) is identified by a complete box and other locations with a dashed line. In the examples below second-order components are in bold type.

a. The location that enables the whole ring system to be named by fusion nomenclature is preferred to one where alternative approaches are required (see FR-7).
Example:

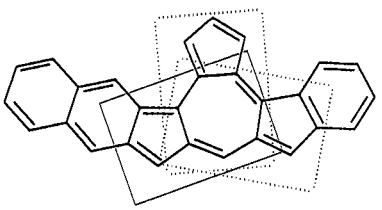


cyclopenta[*ij*]pentaleno[2,1,6-*cde*]azulene
not 1,9-methenopentaleno[1,6-*ef*]azulene
nor 1,9-methenodicyclopenta[*cd*,*f*]azulene

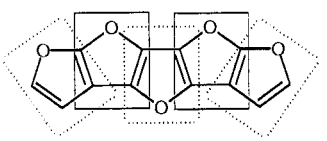
Note With this criterion *CAS* and *Beilstein* permit the use of a less preferred parent component or attached component if that enables the whole system to be named by fusion nomenclature (See however FR-7.1 and FR-7.1.1).

b. The location that results in a name which does not require higher-order attached components. Second order component names are shown in bold below.

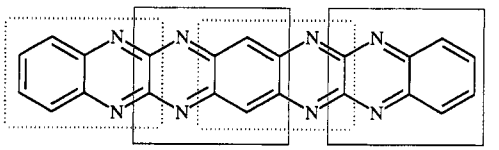
Examples:



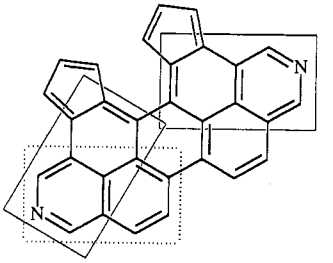
cyclopenta[*h*]indeno[2,1-*f*]naphtho[2,3-*a*]azulene
not benzo[*a*]**benzo**[5,6]indeno[2,1-*f*]cyclopenta[*h*]azulene
nor **benzo**[5,6]indeno[1,2-*e*]indeno[2,1-*h*]azulene
(no second-order components in preferred name)



difuro[3,2-*d*:3',2'-*d*']furo[3,2-*b*:4,5-*b*']difuran
not bis(**furo**[3',2':4,5]furo)[3,2-*b*:2',3'-*d*]furan
nor **furo**[2",3":4,5;5",4":4',5']difuro[2,3-*b*:2',3'-*b*']difuran
(no second-order components in preferred name)



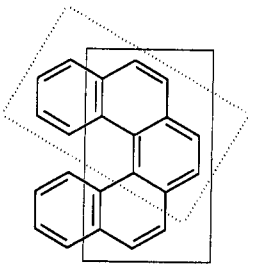
quinoxalino[2,3-*b*]pyrazino[2,3-*g*:5,6-*b'*]diquinoxaline
not quinoxalino[2,3-*b*]**quinoxalino**[2',3':5,6]pyrazino[2,3-*g*]quinoxaline
nor **quinoxalino**[2",3":5',6']**pyrazino**[2',3':6,7]quinoxalino[2,3-*b*]quinoxaline
(no second-order components in preferred name)



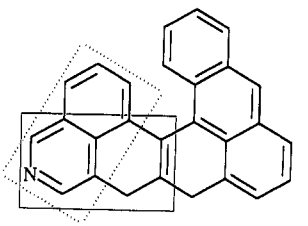
dicyclopenta[*h,h'*]phenanthro[2,1,10-*def*:7,8,9-*d'e'f'*]diisoquinoline
not cyclopenta[*h*]**cyclopenta**[7,8]anthra[2,1,9-*def*:6,5,10-*d'e'f'*]diisoquinoline
(no second-order components in preferred name)

c. The location that results in the maximum number of first-order attached components (then second-order *etc.*).

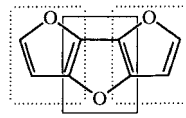
Examples:



dibenzo[*c,g*]phenanthrene
not naphtho[2,1-*c*]phenanthrene
(2 attached components preferred to 1)



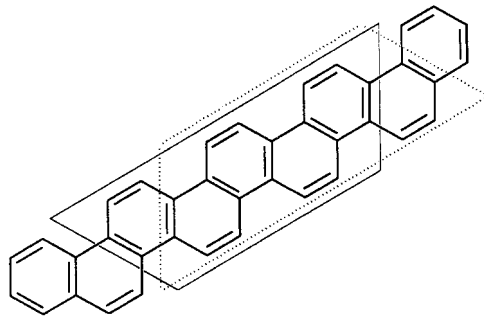
benzo[*de*]**benzo**[1,10]phenanthro[4,3-*g*]isoquinoline
not **naphtho**[3',2',1':8,9]anthra[3,2,1-*de*]isoquinoline
nor di**benzo**[5,6:8,9]phenanthro[2,3,4-*de*]isoquinoline
(2 first-order attached components preferred to 1)



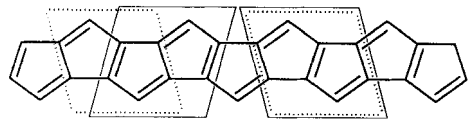
difuro[3,2-*b*:2',3'-*d*]furan
not furo[3,2-*b*:4,5-*b*']difuran
(2 attached components preferred to 1)
(multiplicative name preferred to multiparent name)

d. A location that permits the expression of the maximum number of identical attached components with multiplicative prefixes.

Example:



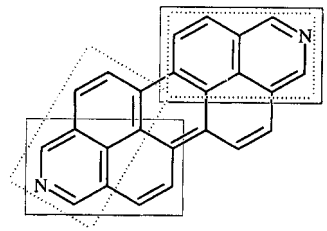
dinaphtho[1,2-*c*:2',1'-*m*]picene
not benzo[*c*]phenanthro[2,1-*m*]picene



1*H*-dipentaleno[2,1-*e*:2',1'-*e*']cyclopenta[1,2-*a*:4,3-*a*']dipentalene
not 1*H*-cyclopenta[*e*]pentaleno[2,1-*e*']pentaleno[2,1-*a*:5,4-*a*']dipentalene

e. A location that uses a preferred interparent component.

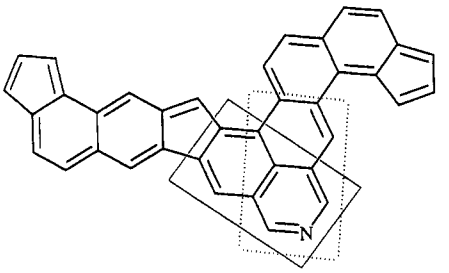
Example:



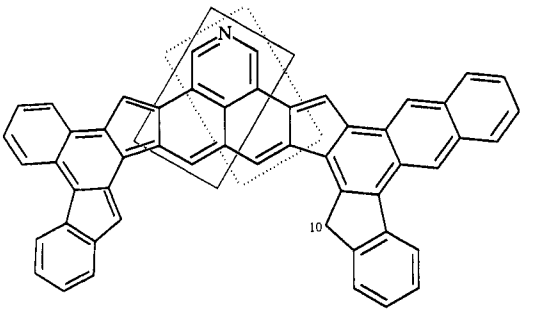
anthra[2,1,9-*def*:6,5,10-*d'e'f'*]diisoquinoline
not phenanthro[2,1,10-*def*:7,8,9-*d'e'f'*]diisoquinoline
(anthracene preferred to phenanthrene)

f. A location that results in preferred attached components (see FR-3.4) comparing first-order attached components, then their attachment locants (see FR-4.5), then comparing the preferred second-order attached components in order of the priority of the first-order components to which they are attached, then their attachment locants (see FR-4.5), then third-order components, *etc.*

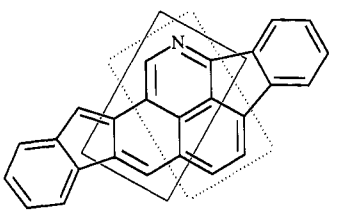
Examples:



cyclopenta[5,6]phenanthro[3,2,1-*de*]**indeno**[4',5':5,6]indeno[2,1-*g*]isoquinoline
not **cyclopenta**[7,8]naphtho[2,1-*g*]**indeno**[5',4':6,7]fluoreno[3,2,1-*de*]isoquinoline
(phenanthrene preferred to fluorene)



10*H*-di**benzo**[4,5:6,7]-*as*-indaceno[1,2-*h*]**indeno**[2',1':5,6]**naphtho**[2',3':7,8]fluoreno-[1,2,3-*de*]isoquinoline
not 10*H*-**benzo**[7,8]**indeno**[2',1':5,6]fluoreno[1,2,3-*de*]**benzo**[6,7]**naphtho**[2',3':4,5]-*as*-indaceno[1,2-*h*]isoquinoline
[at first-order level both names have fluorene[1,2,3-*de*] and *as*-indacene[1,2-*h*] with the same attachment locants, however fluorene is preferred to *as*-indacene;
comparing the preferred second-order component attached to fluorene in each case naphthalene (preferred to indene) is preferred to indene (preferred to benzene)]

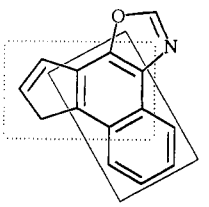


fluoreno[9,1,2-*cde*]indeno[1,2-*h*]isoquinoline
not fluoreno[1,2,3-*de*]indeno[1,2,3-*ij*]isoquinoline
(*cdeh* preferred to *deij*)

FR-3.4 **Selection of attached component(s)**

After selection of the parent component (or parent components and interparent component(s) if a multiparent name is selected - see FR-6) other rings are identified as far as possible as attached components. If there are alternative first-order attached components FR-2.3 is used to select the preferred component.

Example:



8*H*-cyclopenta[3,4]naphtho[1,2-*d*][1,3]oxazole
not 8*H*-benzo[6,7]indeno[5,4-*d*][1,3]oxazole
(naphthalene preferred to indene)

If there are alternative locations for the first-order attached components, the criteria of FR-3.4.1 are used to select the preferred arrangement. After selection of the first-order attached components remaining rings are considered for second-order attached components and so on to higher-order attached components.

If there are alternative names which only differ in their fusion locants see FR-4.5 for the criteria to select the preferred name.

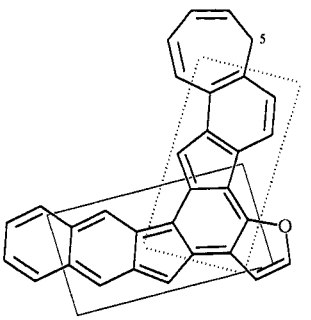
Note Heterobicyclic components with a benzene ring named by FR-2.2.8 are only identified after this stage (see FR-3.5).

FR-3.4.1 *Order of preference between attached components*

If after consideration of the parent component there are two or more potential attached components, or two or more locations for an attached component, the following criteria are applied in order until a distinction is obtained. If a partial distinction is obtained the following criteria are only applied to distinguish between remaining choices. In the examples below the preferred attached component is marked with a complete box and the other location(s) with a dashed line.

a. The location that has preferred locants for fusion to the parent component as a set.

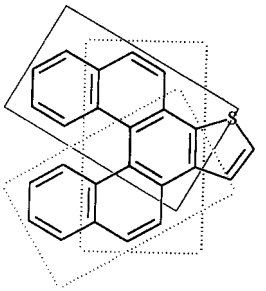
Example:



5*H*-benzo[6,7]cyclohepta[4',5']indeno[1',2':3,4]fluoreno[2,1-*b*]furan
not 5*H*-benzo[5',6']indeno[1',2':1,2]cyclohepta[7,8]fluoreno[4,3-*b*]furan
(1,2 preferred to 3,4)

b. The location that has preferred locants for fusion to the parent component in the order of citation.

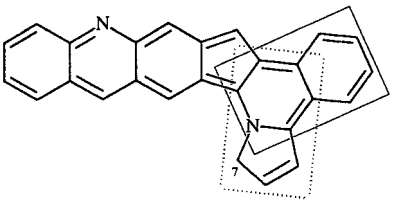
Example:



naphtho[2',1':3,4]phenanthro[1,2-*b*]thiophene
not naphtho[2',1':3,4]phenanthro[2,1-*b*]thiophene
nor dibenzo[3,4:5,6]phenanthro[9,10-*b*]thiophene
(1,2 preferred to 2,1 and both preferred to 9,10)

c. The above procedure is continued exploring outwards to the preferred second-order attached components; preferred fusion locants between the first and second-order attached components; *etc.*

Example:

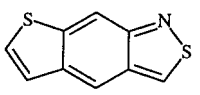


7*H*-pyrrolo[2",1":1',2']isoquinolino[4',3':4,5]cyclopenta[1,2-*b*]acridine
not 7*H*-benzo[7',8']indolizino[6',5':4,5]cyclopenta[1,2-*b*]acridine
(isoquinoline preferred to indolizine)

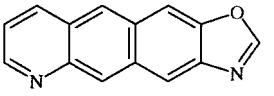
FR-3.5 **Heterobicyclic compounds with a benzene ring as a component**

If the initially identified preferred components for naming the fused ring system include an isolated benzo component (*i.e.* not forming part of a component such as quinoline or naphthalene) *ortho*-fused to a heteromonocyclic component, these two components are treated together as a one-component unit (a 'benzoheterocycle'; see FR-2.2.8). However this approach should not be used if it disrupts a multiparent name (see FR-6) or the use of multiplicative prefixes (FR-4.9). The other initially identified preferred components should not be changed in any other way except in so far as the 'benzoheterocycle' may change the preference between components *i.e.* the use of a 'benzoheterocycle' component may change the order of attached components and may affect the choice of the preferred parent and/or attached component.

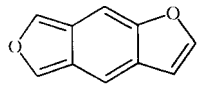
Examples:



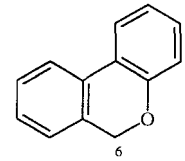
thieno[3,2-*f*][2,1]benzothiazole
(2,1-benzothiazole is preferred to 1-benzothiophene)
CAS name thieno[3,2-*f*]-2,1-benzisothiazole
Beilstein name thieno[3',2':4,5]benzo[1,2-*c*]isothiazole



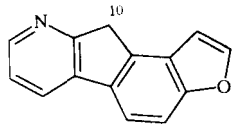
[1,3]benzoxazolo[6,5-*g*]quinoline
(quinoline preferred to benzoxazole)
CAS name benzoxazolo[6,5-*g*]quinoline
Beilstein name oxazolo[4',5':4,5]benzo[1,2-*g*]quinoline



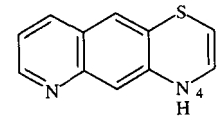
benzo[1,2-*b*:4,5-*c*']difuran
not furo [3,4-*f*][1]benzofuran
(multiparent name preferred)



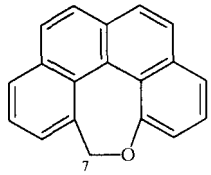
6*H*-benzo[*c*]chromene
CAS name 6*H*-dibenzo[*b*,*d*]pyran



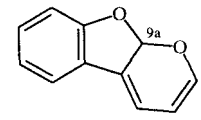
10*H*-furo[3',2':4,5]indeno[2,1-*b*]pyridine
not [1]benzofuro[5',4':3,4]cyclopenta[1,2-*b*]pyridine
(pyridine preferred to benzofuran)
(indene must be used as a component)



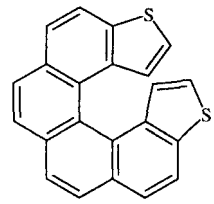
4*H*-[1,4]thiazino[2,3-*g*]quinoline
not 4*H*-pyrido[2,3-*g*][1,4]benzothiazine
(quinoline must be used as a component)



7*H*-phenanthro[5,4,3-*cdef*][1]benzoxepine
Beilstein name 8*H*-1,12-etheno-benzo[*e*]naptho[1,8-*bc*]oxepine



9a*H*-pyrano[2,3-*b*][1]benzofuran
(pyran preferred to furan but
benzofuran preferred to pyran)
CAS name 9a*H*-pyrano[2,3-*b*]benzofuran
Beilstein name 9a*H*-benzo[4,5]furo[2,3-*b*]pyran

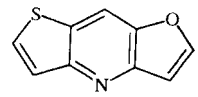


thieno[3',2':5,6]phenanthro[4,3-*e*][1]benzothiophene
CAS name naphtho[1,2-*e*:8,7-*e*']bis[1]benzothiophene
Beilstein name thieno[2",3";5',6']benzo[1',2';5,6]phenanthro[3,4-*b*]thiophene

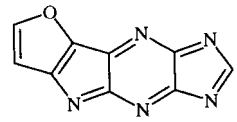
FR-3.6 **Order of citation of fusion prefixes**

Fusion between two components is indicated by the technique described in FR-4. All attached components are cited in front of the parent component(s). Each second-order attached component is cited in front of the first-order attached component to which it is fused and so on to higher-order attached components. If there are two or more different components, or sets of components, attached to a lower-order component they are cited in alphabetical order.

Examples:



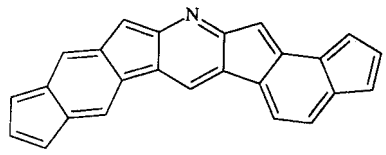
furo[3,2-*b*]thieno[2,3-*e*]pyridine
(**f**uro is before **t**hieno)



furo[2',3':4,5]pyrrolo[2,3-*b*]imidazo[4,5-*e*]pyrazine
(**f**uro-pyrrolo is before **i**midazo)

If the only distinction is between *as*-indacene and *s*-indacene then the italic characters are considered; otherwise they are treated as indacene for consideration of alphabetical order.

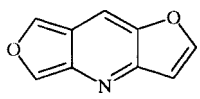
Example:



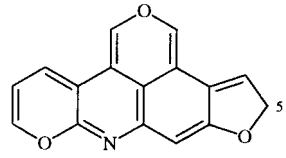
as-indaceno[2,3-*b*]-*s*-indaceno[1,2-*e*]pyridine

If two (or more) identical components are fused to a third they are cited together by the use of di- (or tri-, *etc.*) or bis- (or tris-, *etc.*) as described in FR-4.9. Use of a multiplicative prefix does not affect the alphabetical order of citation of components attached at the same level.

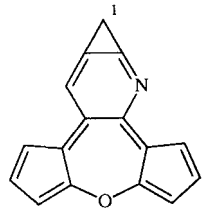
Examples:



difuro[3,2-*b*:3',4'-*e*]pyridine



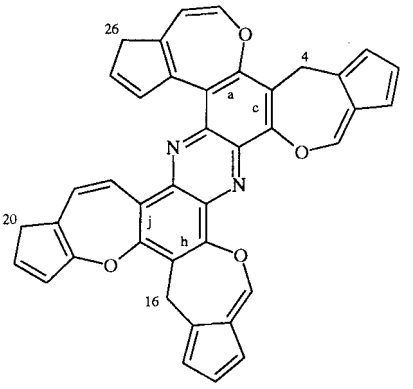
5*H*-furo[3,2-*g*]dipyrano[2,3-*b*:3',4',5'-*de*]quinoline
(**f**uro before di**p**yrano)



1*H*-cyclopropa[*b*]dicyclopenta[2,3:6,7]oxepino[4,5-*e*]pyridine
not 1*H*-dicyclopenta[2,3:6,7]oxepino[4,5-*b*]cyclopropa[*e*]pyridine
[**c**yclopropa is before **d**icyclopentaoxepino (treated as a unit)]

If two or more groups of components only differ by virtue of the fusion locants within the group then these are used to determine the order.

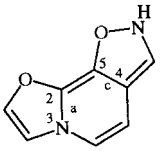
Example:



4*H*,16*H*,20*H*,26*H*-cyclopenta[4,5]oxepino[3,2-*a*]bis(cyclopenta[5,6]oxepino)-[3',2'-*c*:2",3"-*h*]cyclopenta[6"',7"']oxepino[2"',3"'-*j*]phenazine

If two or more groups of components only differ by virtue of the heteroatom locants these are used to determine the order.

Example:



2*H*-[1,2]oxazolo[5,4-*c*][1,3]oxazolo[3,2-*a*]pyridine

FR-4 Fusion Descriptors

After identification of components the fusion name can be constructed. Details of how the common bonds are specified are given below. Examples are labelled, where appropriate, with the relevant letters or locants of components within the rings, and with the numbering of the whole ring system (see FR-5) outside the structure.

FR-4.1 Identification of sides of parent components

The sides around the periphery of the parent component are identified by italic letters *a*, *b*, *c*, *etc.* with *a* for the side 1,2; *b* for the side 2,3 (or in certain cases 2,2a *e.g.* acenaphthylene); *etc.* following continuously round the periphery, ignoring non-standard numbering (see Appendices 1 and 2). If there are more than twenty-six sides the additional sides are identified by subscript numbers a_1, b_1, c_1, *etc.* then a_2, b_2, c_2, *etc.* (Contrast the use of *a'*, *b'*, *c'*, *etc.* in FR-6.1) Each letter locant implies also a direction for the specified bond, *i.e.* the direction of the side *a* is from the atom with locant 1 to the atom with the next higher locant (see arrows on the structures below).

FR-4.2 Identification of sides of attached components

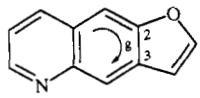
The sides of attached components are identified by the appropriate pairs of number locants.

FR-4.3 Fusion of a first-order attached component to the parent component

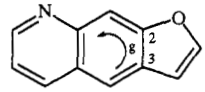
Those bonds that are common to each component are indicated by the appropriate numerical locants for the attached components and letter locants for the parent component separated by a hyphen and cited within square brackets. Numerical locants are separated by commas, while letter locants are quoted together if there is more than one. Letter locants are cited in the same direction as they were assigned (*i.e.* clockwise when considered as in Appendices 1 and 2). The numerical locants are cited in the same direction as the letter locants. The first-order attached component is quoted before the locant set to which it applies and in front of the parent component name. If there is more than one first-order attached component they are quoted in

alphabetical order unless second-order attached components modify this order (see FR-3.6 and FR-4.4). See FR-4.6 for the omission of locants.

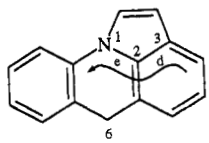
Examples:



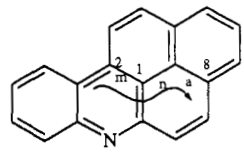
furo[2,3-*g*]quinoline



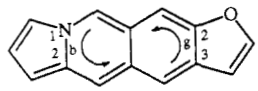
furo[3,2-*g*]quinoline



6*H*-pyrrolo[3,2,1-*de*]acridine



naphtho[2,1,8-*mna*]acridine

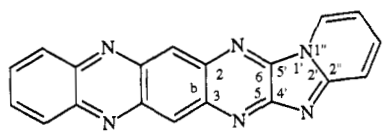


furo[3,2-*g*]pyrrolo[1,2-*b*]isoquinoline

FR-4.4 **Fusion of a higher-order component to an attached component**

The procedure for indicating the common bond(s) between a higher-order attached component and an attached component follows that for the attachment of the first-order attached component to the parent component (see FR-4.3) except that ony numerical locants are used instead of letters and the two sets of locants are separated by a colon. The locants of second-order attached components are primed to contrast with those of first-order attached components. The locants of third-order (fourth-order, *etc.*) attached components are double (triple, *etc.*) primed.

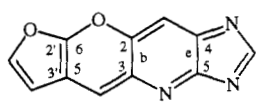
Example:



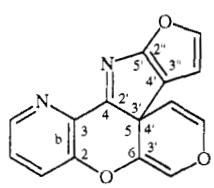
pyrido[1",2":1',2']imidazo[4',5':5,6]pyrazino[2,3-*b*]phenazine

If more than one component is fused to the same lower-order component they are cited in alphabetical order unless higher-order components alter this order (see FR-3.6).

Example:



furo[3',2':5,6]pyrano[3,2-*b*]imidazo[4,5-*e*]pyridine
(**f**uro-pyrano before **i**midazo)



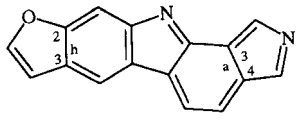
furo[3",2":4',5']pyrrolo[2',3':4,5]pyrano[4',3':5,6]pyrano[3,2-*b*]pyridine
(**f**uro-pyrrolo before **p**yrano)

FR-4.5 **Choice of locants**

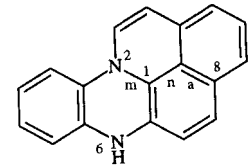
If there is a choice of numerical or letter locants (consistent with the numbering of the component) then the lower numbers or letters are selected. Preference is given in the following order:

a. Parent component letters as a set.

Examples:



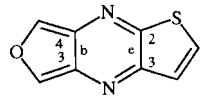
furo[3,2-*h*]pyrrolo[3,4-*a*]carbazole
not furo[2,3-*b*]pyrrolo[3,4-*i*]carbazole
(*a*,*h* preferred to *b*,*i*)



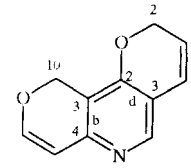
6*H*-isoquinolino[2,1,8-*mna*]phenazine
not 6*H*-isoquinolino[8,1,2-*cde*]phenazine
(*a*,*m*,*n* preferred to *c*,*d*,*e*)

b. Parent component letters in order of citation.

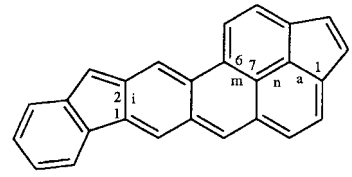
Examples:



furo[3,4-*b*]thieno[2,3-*e*]pyrazine
not furo[3,4-*e*]thieno[2,3-*b*]pyrazine
(*b*....*e* preferred to *e*....*b*)



2*H*,10*H*-dipyrano[4,3-*b*:2',3'-*d*]pyridine
not 2*H*,10*H*-dipyrano[2,3-*d*:4',3'-*b*]pyridine
(*b*....*d* preferred to *d*....*b*)

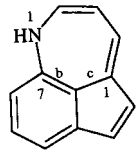


diindeno[1,2-*i*:6',7',1'-*mna*]anthracene
not diindeno[6,7,1-*mna*:1',2'-*i*]anthracene
(*i* ...*mna* preferred to *mna*...*i*)

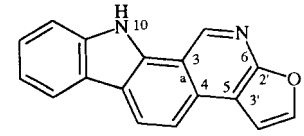
Note Both names for this example have the letters *a*,*i*,*m*,*n* when compared in alphabetic order (see FR-4.5.a), but when compared in the order of citation *i* ...*mna* is preferred to *mna*...*i*.

c. Set of locants for the first-order attached components for fusion to the parent component.

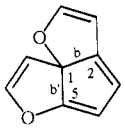
Examples:



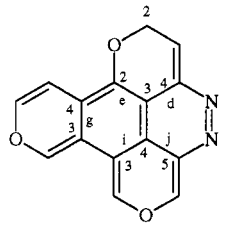
1*H*-indeno[7,1-*bc*]azepine
not 1*H*-indeno[4,3-*bc*]azepine
(1,7 preferred to 3,4)



10*H*-furo[3',2':5,6]pyrido[3,4-*a*]carbazole
not 10*H*-furo[2',3':2,3]pyrido[5,4-*a*]carbazole
(3,4 preferred to 4,5)



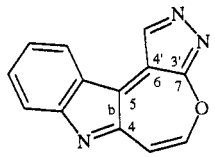
cyclopenta[1,2-*b*:5,1-*b*']difuran
not cyclopenta[1,2-*b*:2,3-*b*']difuran
(1,1,2,5 preferred to 1,2,2,3)



2*H*-tripyrano[4,3,2-*de*:4',3'-*g*:3",4",5"-*ij*]phthalazine
not 2*H*-tripyrano[3,4,5-*de*:3',4'-*g*:2",3",4"-*ij*]phthalazine
(2,3,3',3",4,4',4",5" preferred to 2",3,3',3",4,4',4",5)

d. First-order attached component locants for fusion to the parent component in order of citation.

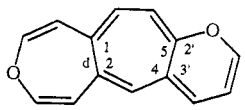
Example:



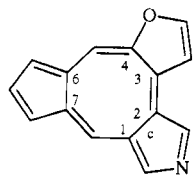
pyrazolo[4',3':6,7]oxepino[4,5-*b*]indole
not pyrazolo[3',4':2,3]oxepino[5,4-*b*]indole
(4,5 preferred to 5,4)

e. Locants for lower-order attached components as a set for fusion to higher-order attached components.

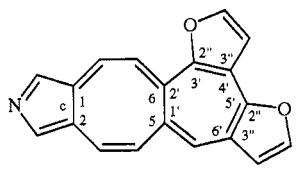
Examples:



pyrano[3',2':4,5]cyclohepta[1,2-*d*]oxepine
not pyrano[2',3':5,6]cyclohepta[1,2-*d*]oxepine
(4,5 preferred to 5,6)



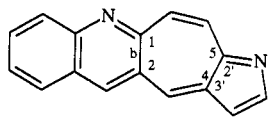
cyclopenta[6,7]furo[3',2':3,4]cycloocta[1,2-*c*]pyrrole
not cyclopenta[4,5]furo[2',3':7,8]cycloocta[1,2-*c*]pyrrole
(3,4,6,7 preferred to 4,5,7,8)



difuro[2",3":3',4';2"',3"':5',6']cyclohepta[1',2':5,6]cycloocta[1,2-*c*]pyrrole
not difuro[3",2":4',5';3"',2"':6',7']cyclohepta[1',2':5,6]cycloocta[1,2-*c*]pyrrole
(3',4',5',6' preferred to 4',5',6',7')

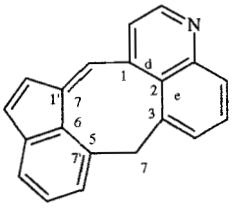
f. Locants for lower-order attached components for fusion to higher-order attached components in order of citation.

Example:



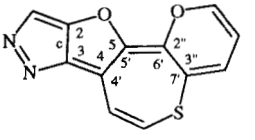
pyrrolo[3',2':4,5]cyclohepta[1,2-*b*]quinoline
not pyrrolo[2',3':5,4]cyclohepta[1,2-*b*]quinoline
(4,5 preferred to 5,4)

g. Locants for higher-order attached components as a set for fusion to the lower-order attached component. Example:



7*H*-indeno[7',1':5,6,7]cycloocta[1,2,3-*de*]quinoline
not 7*H*-indeno[3',4':5,6,7]cycloocta[1,2,3-*de*]quinoline
(1',7' preferred to 3',4')

h. Locants for higher-order components for fusion to lower-order components in order of citation. Example:



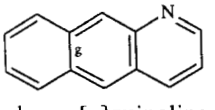
pyrano[2",3":6',7']thiepino[4',5':4,5]furo[3,2-*c*]pyrazole
not pyrano[3",2":2',3']thiepino[5',4':4,5]furo[3,2-*c*]pyrazole
(4',5' preferred to 5',4')

FR-4.6 **Omission of locants**

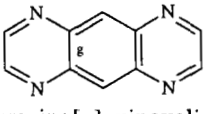
FR-4.6.1 *Unnecessary locants*

If there is no ambiguity the numerical and/or letter locants may be omitted for a system with only first-order attached components.

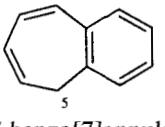
Examples:



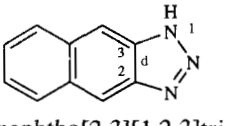
benzo[*g*]quinoline



pyrazino[*g*]quinoxaline
CAS and *Beilstein* name pyrazino[2,3-*g*]quinoxaline



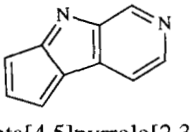
5*H*-benzo[7]annulene
CAS and *Beilstein* name 5*H*-benzocycloheptene



1*H*-naphtho[2,3][1,2,3]triazole
CAS name 1*H*-naphtho[2,3-*d*]triazole
Beistein name 1*H*-naphtho[2,3-*d*][1,2,3]triazole

Locants are also omitted when there is no ambiguity for the fusion of terminal attached components.

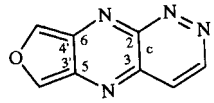
Example:



cyclopenta[4,5]pyrrolo[2,3-*c*]pyridine

When locants are required for the fusion of a higher-order component then all locants for the linking component must be cited.

Example:

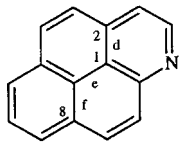


furo[3',4':5,6]pyrazino[2,3-*c*]pyridazine

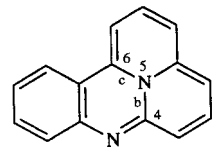
FR-4.6.2 *Locants of peripheral fusion carbon atoms of a component*

The numerical locants of peripheral fusion carbon atoms of a component are omitted with an *ortho-* and *peri-*fused system.

Examples:



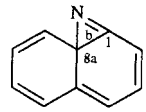
naphtho[2,1,8-*def*]quinoline



quinolizino[4,5,6-*bc*]quinazoline

Both terminal fusion atom locants for *ortho*-fusion must be cited even if one is a fusion atom.

Example:



naphtho[1,8a]azirine

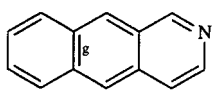
FR-4.7 **Elision**

Vowels are not elided in fusion names, however see FR-2.2.8.

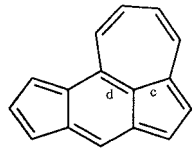
Note The previous edition of these rules included elision (see footnote to A-21.4 ref 3) which is still used by *CAS*. in the following way.

When acenaphtho-, benzo-, or naphtho- is followed by a component which starts with a vowel the 'o' is elided. Similarly the 'a' of cycloalka- is elided under these conditions. In all other cases the 'o' or 'a' is retained.

Examples:



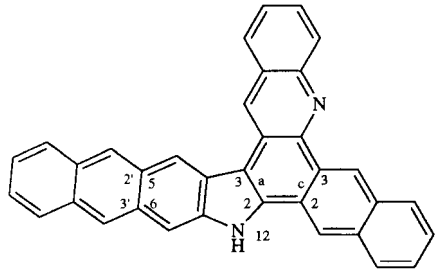
CAS name benz[*g*]isoquinoline
IUPAC name benzo[*g*]isoquinoline



CAS name cyclohept[*cd*]-*s*-indacene
IUPAC name cyclohepta[*cd*]-*s*-indacene

If there is more than one first-order attached component, and at least one second-order attached component, elision between the second-order and the first-order attached component is applied after determination of the alphabetical order of the components (see FR-3.6).

Example:

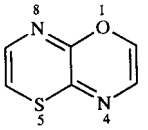


CAS name 12*H*-naphtho[2,3-*c*]naphth[2',3':5,6]indolo[3,2-*a*]acridine
even though naphthindolo is alphabetically before naphtho
IUPAC name 12*H*-naphtho[2,3-*c*]naphtho[2',3':5,6]indolo[3,2-*a*]acridine

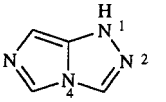
FR-4.8 **Heteroatom locants of components**

When a component requires the citation of locants (*e.g.* in a Hantzsch-Widman name) these are always quoted in square brackets. Note that these numbers in brackets only refer to the numbering of the component and have no significance in the final numbering of the complete fused ring system.

Examples:



[1,4]thiazino[3,2-*b*][1,4]oxazine



1*H*-imidazo[5,1-*c*][1,2,4]triazole

Note In the previous version of these rules (See B-3.1, ref 3) any locants of a component which are cited in the name and are the same as that of the final system (see FR-5.3 and FR-5.4) are not enclosed in brackets.

CAS still does not use brackets when the locants of the heteroatoms of the component correspond to those of the whole fused ring system. Thus the *CAS* index names for the above examples are [1,4]thiazino[3,2-*b*]-1,4-oxazine and 1*H*-imidazo[5,1-*c*]-1,2,4-triazole although in the latter case the triazole was numbered anticlockwise to derive the fusion locants and clockwise afterwards to assign the system locants.

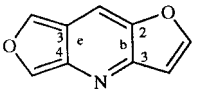
FR-4.9 **Treatment of identical attached components**

When there are two or more components which are identical and both fused to a parent or attached component this is indicated by the use of the prefix di-, tri-, *etc.* (or bis-, tris-, *etc.* to avoid ambiguity). This multiplicative prefix is not considered in deciding the alphabetical order of components attached at the same level (see FR-3.6).

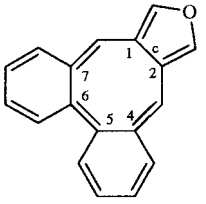
If a complete set of locants are used for first-order attached components fused to the parent component these are cited together separated by a colon. If abbreviated sets of locants are used the letters are separated by a comma. If complete sets of locant are used for second-order attached components fused to a first-order attached component, or for higher-order cases, the locants are cited together separated by a semicolon. If abbreviated sets are used they are separated by a colon. (See note 1)

To distinguish between the two or more components of the same order the locants of the second component are primed (or double primed if the first is primed, *etc.*), the third double primed *etc.*

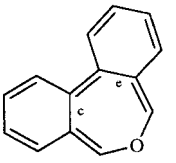
Examples:



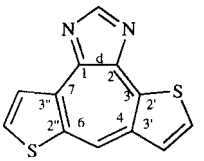
difuro[3,2-*b*:3',4'-*e*]pyridine



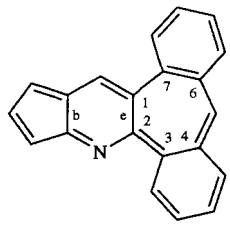
dibenzo[4,5:6,7]cycloocta[1,2-*c*]furan



dibenzo[*c*,*e*]oxepine



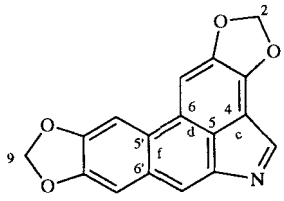
dithieno[2',3':3,4;2",3":6,7]cyclohepta[1,2-*d*]imidazole



cyclopenta[*b*]dibenzo[3,4:6,7]cyclohepta[1,2-*e*]pyridine

If the use of di-, tri-, *etc*. might be ambiguous bis-, tris-, *etc*. are used. This applies when di-, tri-, *etc*. prefixes might be used to name the component (*e.g.* Hantzsch-Widman name).

Example:



2*H*,9*H*-bis[1,3]benzodioxolo[4,5,6-*cd*:5',6'-*f*]indole

Beilstein name [1,3]dioxolo[4',5':4,5]benzo[1,2-f][1,3]dioxolo[4',5':5,6]benzo[1,2,3-*cd*]indole

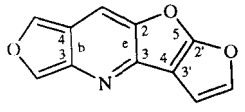
Notes 1. Apart from the use of a hyphen with a full set of locants for fusion of the first-order attached component to a parent component the punctuation is in the order comma, colon, semicolon. See examples above. The semicolon separates sets which use a colon; the colon separates sets which use a comma or hyphen; and the comma is used if only one punctuation mark is needed.

Beilstein uses the hyphen as above. A colon is used for fusion of attached components. A semicolon is used to separate fusion descriptors which already contain a colon or comma *e.g.* difuro[3,2-*b*;3',4'-*e*]pyridine and dibenzo[4,5;6,7]cycloocta[1,2-*c*]furan (*cf.* above).

FR-4.9.1 *Additional components attached to a system with a multiplicative prefix*

Fusion of a higher-order attached component to a system named with a multiplicative prefix requires each set of attached components to be specified separately.

Example:

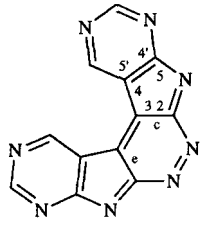


furo[3,4-*b*]furo[3',2':4,5]furo[2,3-*e*]pyridine

FR-4.9.2 *Groups of identical components with identical fusion*

When two or more groups of identical components (including identical fusion between these components) are fused to another component this is indicated by the use of bis-, tris-, *etc*. with the group of components in round brackets.

Example:



bis(pyrimido[5',4':4,5]pyrrolo)[2,3-*c*:3',2'-*e*]pyridazine

CAS name bispyrimido[5',4':4,5]pyrrolo[2,3-*c*:3',2'-*e*]pyridazine

FR-5 Numbering

The older rules for numbering fused ring systems (ref 2) were based on the concept of converting all systems into an approximate two-dimensional hexagonal grid framework. As the complexity of fused ring systems increased these arbitrary rules have been extended as needed. It is recognised that there are problems which are not covered by this document with some systems containing three-membered rings or with rings greater than seven.

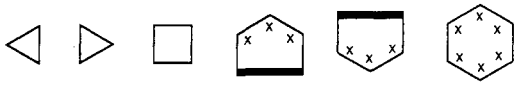
Note All ring systems in this document have been drawn so that the peripheral numbering (not always shown) is clockwise and starts approximately in the top right hand ring.

FR-5.1 Drawing of fused ring system for orientation

Before the fused ring system can be orientated it must be drawn according to the following specifications. If more than one drawing meets these specifications the one chosen is that which gives the more preferred orientation (FR-5.2) and if there is still a choice the more preferred numbering (FR-5.3).

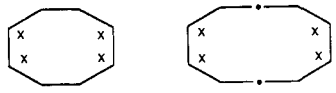
FR-5.1.1 *Allowable shapes for component rings in the horizontal row*

In the preferred orientation of a ring system, as many rings as possible should be in the same horizontal row (FR-5.2.a). Permitted shapes for three- to six-membered rings which form the horizontal row are:

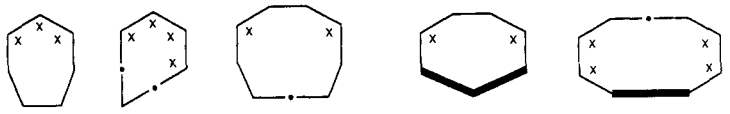


The five-membered ring may be considered as a six-membered ring with one atom eliminated and replaced by an elongated bond (shown thickened above). Internal ring angles of 120° are marked with an 'x'.

Rings with an even number of members greater than six are considered as modified six-membered rings with additional pairs of horizontal bonds inserted between the two halves. This arrangement ensures that rings fused on both sides in the horizontal row are fused to bonds as far apart as possible. For eight- and ten-membered rings permitted shapes are:

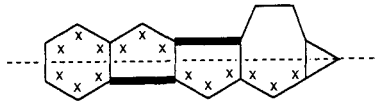


A ring with an odd number of members greater than six is considered as a modification of the corresponding even membered ring with one more or less member above or below so that rings fused on both sides in the horizontal row are fused to bonds as far apart as possible. For the seven- and nine-membered rings permitted shapes are:



The three left-hand forms correspond to insertion into a smaller ring with one less member. The two right-hand forms correspond to deletion from larger rings with one more member. In each case the rings may also be orientated with the modified region at the top instead of the bottom.

Example:

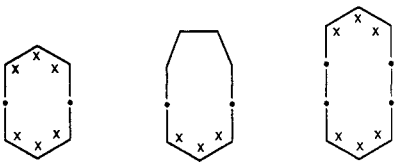


(axis of horizontal row shown by dotted line)

FR-5.1.2 *Allowable shapes for other component rings*

Rings ortho- or ortho- and peri-fused to the horizontal row may also be drawn as shown in FR-5.1.1 but other shapes or orientations are permitted. With a five-membered ring the shape may need to be orientated as follows:

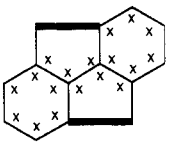
Additional modifications of rings with more than seven members are permitted. For eight-, nine- and ten-membered rings permitted shapes are:



These modifications may be required for fusion to the horizontal row (see FR-5.3 example 3), or, if additional rings are fused above or below the nine- or ten-membered rings, they may need to be used for rings in the main horizontal row provided the rings on either side in the horizontal row are fused to bonds as far apart as possible (i.e. to the bond with a dot at each end for a ten-membered ring).

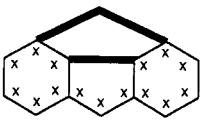
In drawing an *ortho-* and *peri*-fusion the individual rings should be orientated so that each internal ring angle involved is 120°. Such angles are marked with an 'x' in the above diagrams. If this is not possible see FR-5.1.5. Elongated bonds, shown thickened in the diagrams above, should not be used for fusion. If this is not possible see FR-5.1.6.

Example:



Only preferred shapes used

not

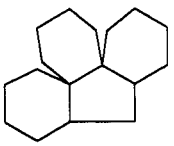


Distorted ring fused to elongated bond

FR-5.1.3 *Overlap of bonds*

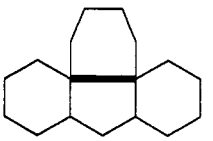
If the fused ring system can be drawn in more than one way using the preferred ring shapes (FR-5.1.1 and FR-5.1.2) preference is given to those forms which do not involve overlap of bonds. If, when using these preferred ring shapes two bonds overlap, it is necessary to draw one (or both) of the rings involving those bonds with a modified shape to show that the two rings are not *ortho*-fused together. This modification is not considered to represent distortion in the sense of FR-5.1.5.

Example:



Only preferred ring shapes used, slightly modified

not

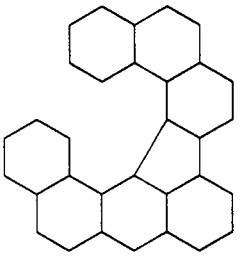


Distorted ring fused to elongated bond

FR-5.1.4 *Overlap of rings*

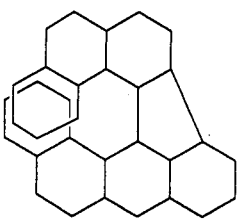
If the fused ring system can be drawn in more than one way using the preferred ring shapes (FR-5.1.1 and FR-5.1.2) preference is given to those forms which do not involve overlap of rings. If, when using these preferred ring shapes two rings overlap, it may be necessary to draw one or more rings with a slight modification to show the two overlapping rings. This modification does not constitute distortion in the sense of FR-5.1.5.

Examples:

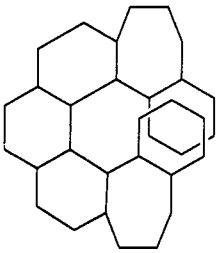


No overlap of rings

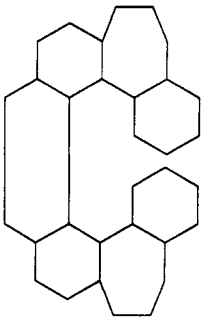
not



Overlap of rings



not



Only preferred shapes used

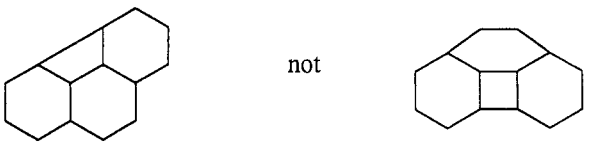
Distorted ring shape

FR-5.1.5 *Distorted ring shapes*

If the fused ring system cannot be drawn using only the above shapes then the minimum number of distorted ring shapes should be used. Where there is a choice distortion of a smaller ring is preferred to distortion of a larger ring. If possible the rings in the horizontal row should not be distorted. The following shapes are quite often required:

The 120° angles marked with an 'x' are suitable for *peri*-fusion. The thickened (elongated bonds) should not be used for fusion.

Example:



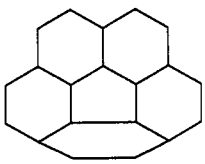
not

Distorted four-membered ring preferred to distorted six-membered ring.

FR-5.1.6 *Fusion to an elongated bond*

If the fused ring system cannot be drawn following FR-5.1.1, FR-5.1.2 or FR-5.1.5 then the minimum number of elongated bonds may be used for fusion. If there is a choice then elongated bonds of a smaller ring are preferred to those of a larger ring.

Example:



FR-5.2 **Orientation**

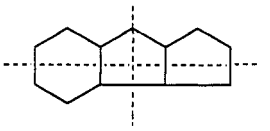
Before the drawing (or drawings if there is more than one of equal preference) is numbered it needs to be orientated. In considering possible orientations it should be remembered that the system can be rotated in the plane of the ring system and can also be turned over. The preferred orientation is established by consideration of the following points in order. If a choice remains, the final decision is made by consideration of the preferred numbering (see FR-5.4).

a. *Maximum number of rings in a horizontal row*

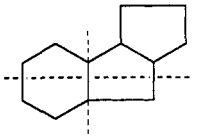
The preferred drawing is that with the greatest number of *ortho*-fused rings, with vertical common bonds, in a horizontal row. The relevant vertical bonds are always those furthest apart. If the correct orientation is not immediately apparent bisect the horizontal row by a horizontal axis and a vertical axis to

form four quadrants. Rings which are bisected by the horizontal axis but are not directly *ortho*-fused to the main row are not considered when counting how many rings are in the row [see example 2 in FR-5.2(b)].

Example:



is preferred to

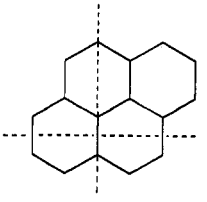


(3 rings in row) (2 rings in row)

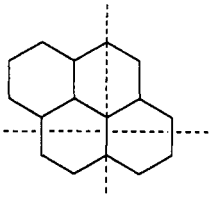
b. *Maximum number of rings in upper right quadrant*

In the preferred orientation, the maximum number of rings should appear above the horizontal row on the right hand side (upper right quadrant). For this purpose the centre of the row is defined as the central common bond if there is an even number of rings in the row, and the centre of the central ring if there is an odd number of rings. When counting rings in a quadrant those rings which are divided by an axis are considered as two halves and the ring at the centre of the row, if bisected by both axes, counts as four quarters.

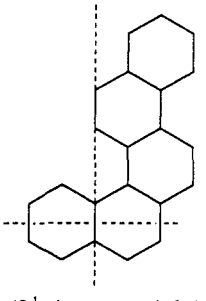
Examples:



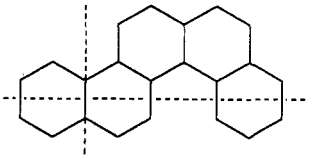
is preferred to



(2 rings top right) (1 ring top right)



is preferred to



($3\frac{1}{2}$ rings top right) (3 rings top right)

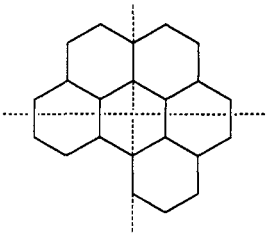
Notes 1. The right hand structure only has two rings *ortho*-fused in a row. The third ring in the row is not directly *ortho*-fused to the other two.

2. Rings are counted in the quadrant in which they are drawn.

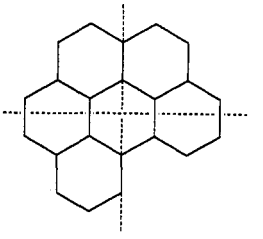
c. *Minimum number of rings in lower left quadrant*

In the preferred orientation the minimum number of rings should appear below the row on the left hand side (lower left quadrant).

Example:



is preferred to

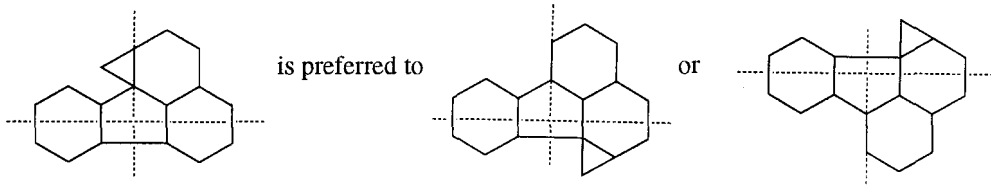


($\frac{3}{4}$ ring lower left) ($1\frac{3}{4}$ rings lower left)

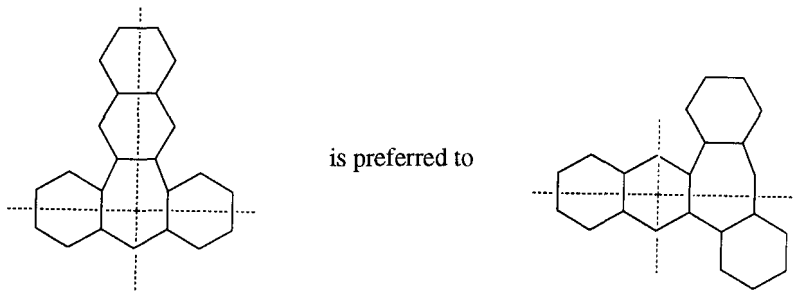
d. *Maximum number of rings above the horizontal row*

In the preferred orientation, the maximum number of rings should appear above the horizontal row identified in FR-5.2(a).

Example:



($3\frac{1}{2}$ rings above row) ($2\frac{1}{2}$ rings above row)



($3\frac{1}{2}$ rings above row) ($2\frac{1}{2}$ rings above row)

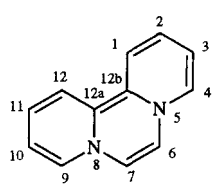
e. *Preferred peripheral numbering*

The preferred orientation is that which gives preferred peripheral numbering (see FR-5.3).

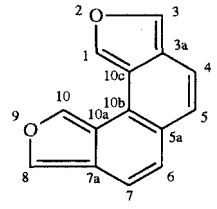
FR-5.3 **Peripheral numbering**

The numbering of the peripheral atoms in a particular orientation starts from the uppermost ring. If there is more than one uppermost ring the ring furthest to the right is chosen. Numbering starts from the non-fusion atom most counterclockwise in the ring selected, and numbering proceeds in a clockwise direction around the system, including fusion heteroatoms. Fusion carbon atoms are not included; each fusion carbon atom is given the same number as the immediately preceding position modified by a roman letter a, b, c, etc. If heteroatoms are identified by replacement nomenclature all atoms retain the numbers of the parent hydrocarbon.

Examples:



dipyrido[1,2-*a*:2',1'-*c*]pyrazine

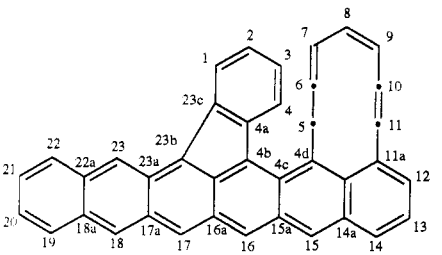


naphtho[1,2-*c*:7,8-*c*']difuran

Note Polyhelicenes are treated differently as an exception to this rule (see FR-2.1.7).

If there are rings of different sizes consideration of the uppermost ring is based on the level above the horizontal row of FR-5.2(a) in the idealised two dimensional hexagonal grid (see start of FR-5) rather than the geometric height above the horizontal row. Rings directly fused to the horizontal row identified in FR-5.2(a) are considered as the first row above the horizontal. The second row above are fused to the first row and so on.

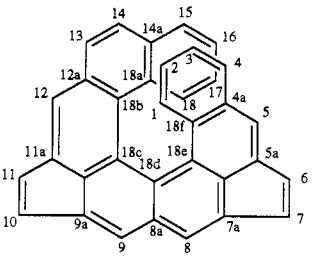
Example:



5*H*-cyclodeca[*de*]indeno[1,2,3-*hi*]hexacene
(The indene six-membered ring is two rows above the horizontal row.)
(The ten-membered ring is only one row above the horizontal row.)

If due to overlap there is still a choice the ring fused to the ring furthest right is chosen.

Example:

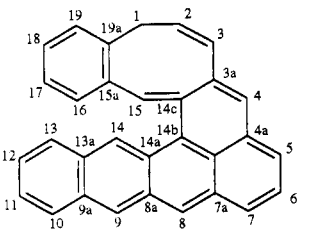


dicyclopenta[*gh*,*mn*]heptahelicene

Note The distortion here is introduced only in order to see each ring clearly.

If there is a choice of starting points numbering starts from the atom most counterclockwise in a continuous non-fusion portion of the ring selected. If there is still a choice of starting points the uppermost one is selected.

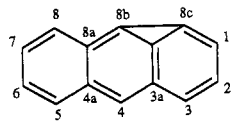
Example:



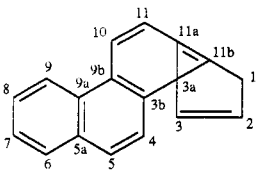
1*H*-benzo[6',7']cycloocta[1',2':4,5]benzo[1,2,3-*de*]tetracene
(numbering does not start at position 15)

If the selected ring does not have a non-fusion atom then numbering starts in the next ring encountered when proceeding round the system in a clockwise direction.

Examples:



cyclopropa[*de*]anthracene



1*H*-cyclopenta[1,3]cyclopropa[1,2-*a*]phenanthrene

Note Cyclopenta[*a*]phenanthrene is numbered as a steroid (ref 12) by *CAS*. In these recommendations it is numbered in the standard way. This is a change from rule A-22.5 (ref 3).

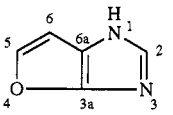
CAS also names and numbers additional cyclopropane rings fused to cyclopenta[*a*]phenanthrene using this numbering *e.g.* cyclopropa[2,3]cyclopenta[*a*]phenanthrene instead of cyclopenta[*a*]cyclpropa[*h*]phenanthrene. This numbering is also used for oxirene and thiirene rings (but not azirine) fused to cyclopenta[*a*]phenanthrene. These rings are indicated by *CAS* using the corresponding bridging prefixes (epoxy and epithio).

FR-5.4 **Order of preference between alternative numbering systems**

If there are alternative orientations of a ring system which are equally preferred after the application of FR-5.2 (including alternative locations for the heteroatoms) then the following rules are applied in order until a preferred numbering of the peripheral atoms is identified.

a. Give low numbers for the heteroatoms as a set.

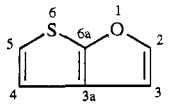
Example:



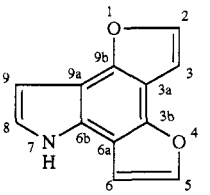
1*H*-furo[2,3-*d*]imidazole
(1,3,4 is preferred to 1,3,6 or 1,4,6)

b. Give low numbers for heteroatoms when considered in the order: O, S, Se, Te, N, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Hg [*i.e.* Table I of the revised Hantzsch-Widman system (ref 9)].

Examples:



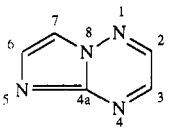
thieno[2,3-*b*]furan



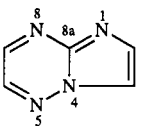
7*H*-difuro[2,3-*e*:2',3'-*g*]indole

c. Give low numbers to fusion carbon atoms.

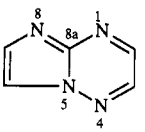
Example:



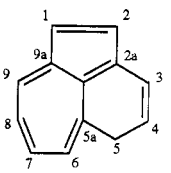
not



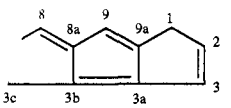
nor



imidazo[1,2-*b*][1,2,4]triazine
(4a is lower than 8a)



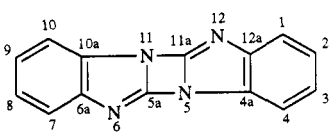
5*H*-benzo[*cd*]azulene
(2a,5a,9a is lower than 2a,6a,9a; 3a,5a,9a; 3a,7a,9a; 4a,6a,9a; or 4a,7a,9a)



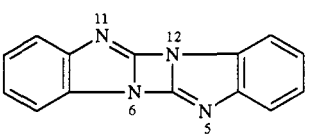
1*H*-cyclopenta[2,1-*a*:3,4-*a*']dipentalene
(3a,3b,3c... preferred to 3a,4a,5a...)

d. Give low numbers to fusion rather than non-fusion atoms of the same heteroelement.

Example:



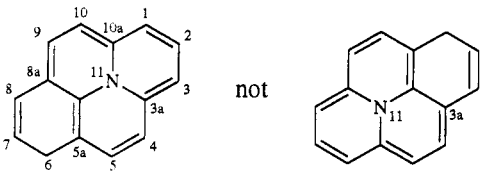
not



[1,3]diazeto[1,2-*a*:3,4-*a*']dibenzimidazole
(5 is preferred to 6)

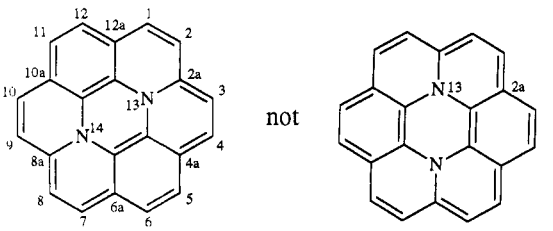
e. Give low numbers so that an internal heteroatom is nearer (*i.e.* less bonds in the pathway) to the lowest numbered fusion peripheral atom.

Example:



6*H*-quinolizino[3,4,5,6-*ija*]quinoline
(11 is 1 bond from 3a)
CAS name 6*H*-benzo[*ij*]pyrido[2,1,6-*de*]quinolizine)

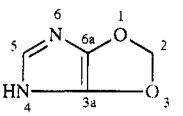
Note In this example the peripheral numbering is determined by the nitrogen atom not by indicated hydrogen.



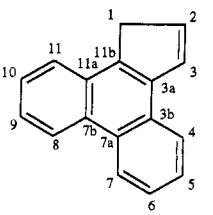
diquinolizino[3,4,5,6,7-*defg*:3',4',5',6',7'-*klmn*]phenazine
(13 is 1 bond from 2a)

f. Give low numbers to indicated hydrogen atoms (expressed or implied).

Example:



2*H*,4*H*-[1,3]dioxolo[4,5-*d*]imidazole
not 2*H*,6*H*-[1,3]dioxolo[4,5-*d*]imidazole



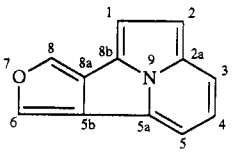
1*H*-cyclopenta[*l*]phenanthrene
not 3*H*-cyclopenta[*l*]phenanthrene

FR-5.5 **Interior numbering**

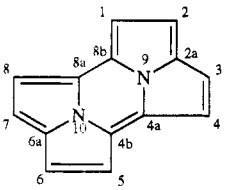
FR-5.5.1 *Heteroatoms*

Interior heteroatoms (not identified by replacement nomenclature) are numbered after the peripheral atoms continuing the number sequence. If there is a choice the shortest path of bonds from each heteroatom to the periphery is determined. The lower number is given to the heteroatom which is closest to the lowest numbered peripheral atom.

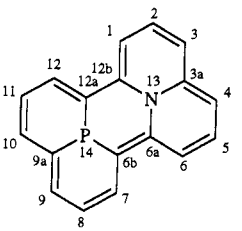
Examples:



furo[3,4-*a*]pyrrolo[2,1,5-*cd*]indolizine



pyrazino[2,1,6-*cd*:3,4,5-*c'd'*]dipyrrolizine
(9 is one bond from 2a)



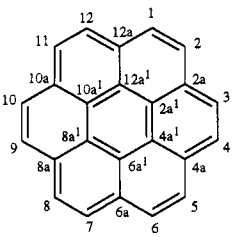
phosphinolizino[4',5',6':3,4,5][1,4]azaphosphinino[2,1,6-*de*]quinolizine
(nitrogen has a lower number than phosphorus, see FR-5.4.b)

Note Previously it was recommended that interior heteroatoms were numbered last following the shortest path from the highest previous number (rule B-3.4.e ref 3).

FR-5.5.2 *Carbon atoms*

Interior carbon atoms are numbered by identifying the minimum number of bonds linking them to the periphery. The locant for the interior atom is that of the peripheral atom with a superscript number corresponding to the number of bonds between the two atoms.

Example:

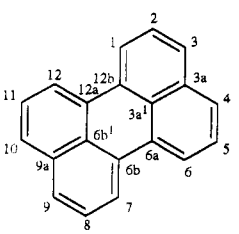


coronene

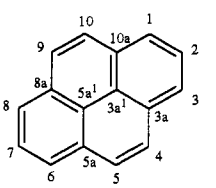
Note Rule A-22.2 recommended that interior atoms follow the highest numbered peripheral atom sequence. For example those in pyrene (below) were numbered 10b and 10c ($3a^1$ and $5a^1$ respectively). *CAS* and *Beilstein* still use this system.

If there is a choice of interior atom locants lower numbers are preferred.

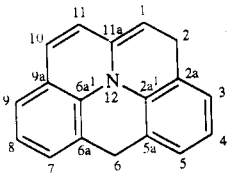
Examples:



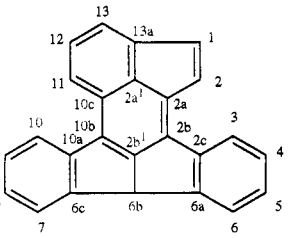
perylene



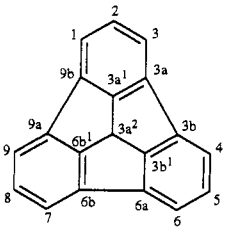
pyrene



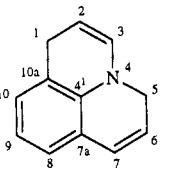
2*H*,6*H*-quinolizino[3,4,5,6,7-*defg*]acridine



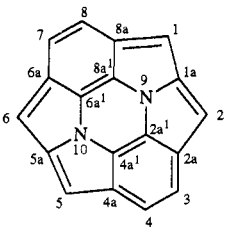
6b*H*-diindeno[1,7-*bc*:1',2',3'-*lm*]fluorene



3a^2*H*-benzo[3,4]pentaleno[2,1,6,5-*jklm*]fluorene



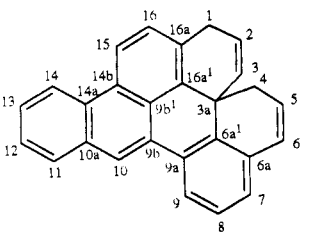
1*H*,5*H*-pyrido[3,2,1-*ij*]quinoline
CAS name 1*H*,5*H*-benzo[*ij*]quinolizine



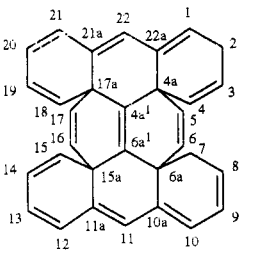
dipyrrolizino[2,3,4,5,6-*defg*:2',3',4',5',6'-*klmn*]phenazine

A non-free spiro peripheral atom is not used as reference for interior carbon atoms, if ambiguity would result. In the first example below carbon atom 3a is a non-free spiro peripheral atom.

Examples:



1*H*,4*H*-dibenzo[*b*,*gh*]perylene



2*H*,7*H*-tetrabenzo[*c*,*g*,*j*,*n*]pyrene

Note If 3a had been used as a reference atom in the first example both 6a^1 and 16a^1 would be 3a^1.

The system described in A-22.2 (ref 3) has been developed by *CAS* to deal with complex examples (See ref 18). Their additional rules to number interior atoms for complex examples are as follows.

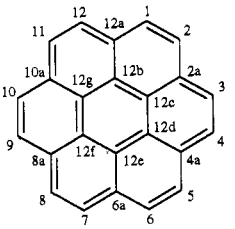
a. Starting from the highest numbered atom (peripheral atom or interior numbered heteroatom) the longest continuous path of interior atoms is determined and numbered by adding the letter 'a', 'b', 'c', *etc.* in turn to that of the highest numbered atom. This procedure is repeated at the next highest numbered atom *etc.* until all interior atoms are numbered.

b. If there are alternative pathways the two alternative atoms at the branch point are compared using the shortest path to the periphery for each atom. The atom linked in this way to the lower numbered peripheral atom is selected.

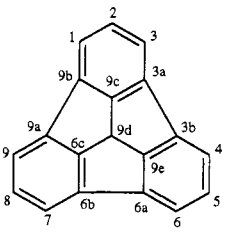
c. Isolated interior atoms and chains not covered by (a) or (b) above are numbered using the longest chain of unnumbered atoms with the numbering continuing from the highest numbered alphanumeric locant available.

d. If there are interior numbered heteroatoms the longest chain of interior atoms attached to the interior heteroatom is numbered as above.

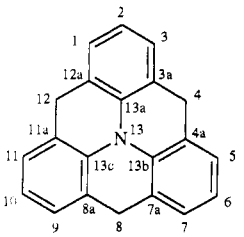
Examples:



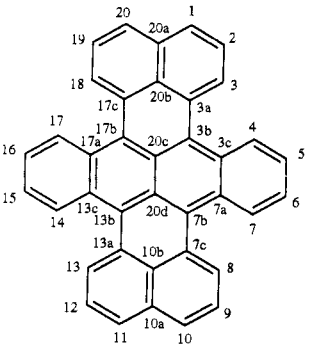
coronene



9d*H*-benzo[3,4]pentaleno[2,1,6,5-*jklm*]fluorene



4*H*,8*H*,12*H*-benzo[1,9]quinolizino[3,4,5,6,7-*defg*]acridine



tribenzo[*de*,*h*,*kl*]naphtho[1,2,3,4-*rst*]pentaphene

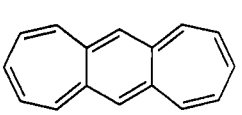
FR-6 Multiparent Systems

When there are two or more non-overlapping locations for the parent component (see FR-3.3) and they are *ortho-* or *ortho-* and *peri*-fused to the same first order interparent component (see FR-1.3.3) they are treated as multiparent system and given a multiparent name. Similarly a system with three, five, seven, *etc.* interparent components is treated as an extended multiparent system. Each pair of second- or higher-order interparent components must be identical.

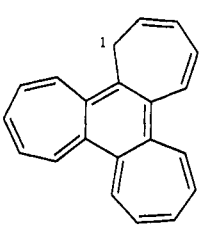
FR-6.1 Multiparent systems with one interparent component

The multiple occurences of the parent component in a multiparent system is indicated by the use of the prefix di-, tri-, *etc.* (or bis-, tris-, *etc.* see FR-4.9). To distinguish between the parent components the second one has primed letters, the third double primed *etc.* and the sets of locant are separated by a colon.

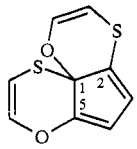
Examples:



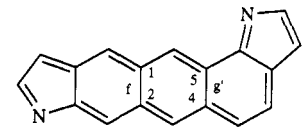
benzo[1,2:4,5]di[7]annulene



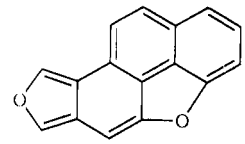
1*H*-benzo[1,2:3,4:5,6]tri[7]annulene



cyclopenta[1,2-*b*:5,1-*b*']bis[1,4]oxathiine



benzo[1,2-*f*:4,5-*g*']diindole

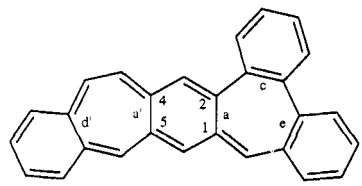


phenanthro[4,5-*bcd*:1,2-*c*']difuran

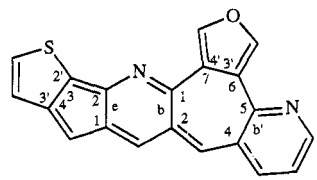
FR-6.2 **Additional attached components**

Additional attached components may be fused to any of the components of a multiparent system. If FR-4.5 does not provide the preferred locants preference is given to the unprimed component and the fusion letters are assigned with the lower letter used for fusion to the connecting component. Great care is needed with the use of primes, double primes *etc.* to ensure that there is no ambiguity. Thus additional components fused to the interparent component(s) are cited next to the prefix for this interparent component.

Examples:



tribenzo[*c*,*d*',*e*]benzo[1,2-*a*:4,5-*a*']di[7]annulene



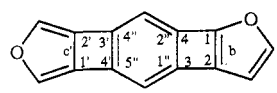
thieno[2',3':3,4]cyclopenta[1,2-*e*]furo[3',4':6,7]cyclohepta[1,2-*b*:5,4-*b*']dipyridine

Note The furan ring is fused to the interparent component so that alphabetic order does not apply.

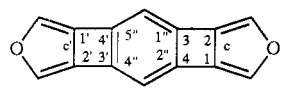
FR-6.3 **Multiparent systems with three or more interparent components**

If two (or more) possible parent components are separated by an odd number of interparent components and these are ordered symmetrically with respect to their component rings (but not necessarily with respect to their fusion locants) the whole system is treated as a multiparent system. Second- and higher-order interparent components are named using the prefix di-, tri-, *etc.* (or bis-, tris-, *etc.* if appropriate).

Examples:

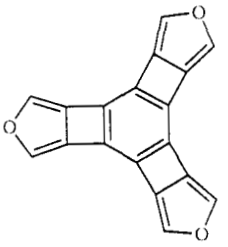


benzo[1",2":3,4;4",5":3',4']dicyclobuta[1,2-*b*:1',2'-*c*']difuran

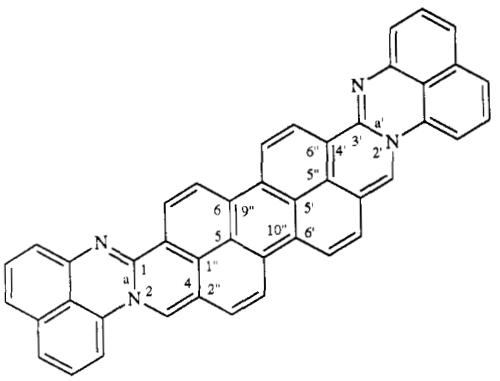


benzo[1",2":3,4;4",5":3',4']dicyclobuta[1,2-*c*:1',2'-*c*']difuran
or benzo[1",2":3,4;4",5":3',4']bis(cyclobuta[1,2-*c*]furan)

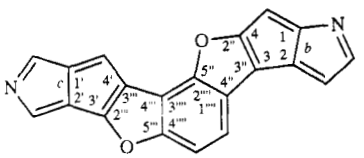
Note This alternative method of naming symmetric systems is not used by *CAS*. *Beilstein* applies it to systems with five or more interparent components.



benzo[1‴,2‴:3,4;3‴,4‴:3',4';5‴,6‴:3",4"]triscyclobuta[1,2-*c*:1',2'-*c*':1",2"-*c*"]trifuran
or benzo[1‴,2‴:3,4;3‴,4‴:3',4';5‴,6‴:3",4"]tris(cyclobuta[1,2-*c*]furan)



anthra[2",1",9":4,5,6;6",5",10":4',5',6']diisoquinolino[2,1-*a*:2',3'-*a*']diperimidine

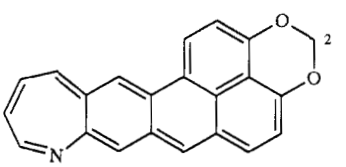


benzo[1"",2"":4",5";3"",4"":4"",5""]difuro[3",2":3,4;2‴,3‴:3',4']dicyclopenta-
[1,2-*b*:1',2'-*c*']dipyrrole

FR-7 Three Components *ortho*- and *peri*-Fused Together

The fusion principles described above only apply between pairs of components. It is not possible to name a system where a third component is *ortho*- and *peri*-fused to two components which are themselves *ortho*- or *ortho*- and *peri*-fused together. To avoid this situation the following procedures are applied in order until a name can be formed. However if one of the three components is a benzene ring and another is a heteromonocycle then application of FR-2.2.8 will sometimes permit normal fusion procedures that would not otherwise be possible.

Example:

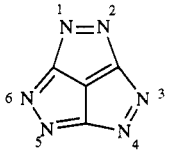


2*H*-[1,3]benzodioxino[6',5',4':10,5,6]anthra[2,3-*b*]azepine

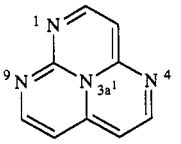
FR-7.1 **Use of replacement nomenclature**

If the corresponding hydrocarbon fused ring system can be named by fusion principles or has a trivial name then the heteroatoms are identified by replacement nomenclature using 'a'-terms.

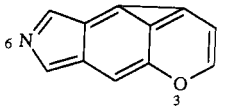
Examples:



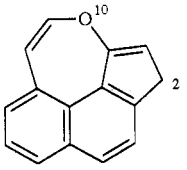
1,2,3,4,5,6-hexaazacyclopenta[*cd*]pentalene



1,3a^1,4,9-tetraazaphenalene
(See FR-5.5.2)
CAS and *Beilstein* name 1,4,9,9b-tetraazaphenalene



3-oxa-6-azacyclopenta[*b*]cyclopropa[*de*]naphthalene
CAS name cyclopropa[4,5][1]benzopyrano[6,7-*c*]pyrrole
Beilstein name cyclopropa[4,5]chromeno[6,7-*c*]pyrrole



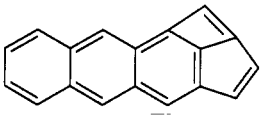
2*H*-10-oxanaphtho[2,1,8-*cde*]azulene
CAS name 1*H*-benzo[*ef*]cyclopenta[*jk*][2]benzoxepine

Note *CAS* and *Beilstein* use less preferred components in preference to replacement if by this device fusion nomenclature can be used. See last two examples above.

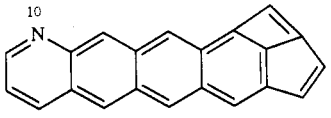
FR-7.1.1 **Use of less preferred parent component**

If the corresponding hydrocarbon fused ring system cannot be named by the fusion principles outlined above then a less preferred parent component is selected which will permit fusion nomenclature to be used.

Examples:



cyclobuta[1,7]indeno[5,6-*b*]naphthalene
not cyclobuta[*cd*]naphtho[2,3-*f*]indene
(naphthalene preferred to indene)

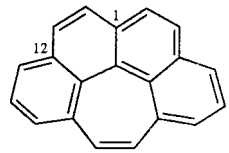


10-azacyclobuta[1,4]indeno[5,6-*b*]anthracene

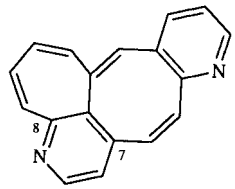
FR-7.2 **Use of bridging nomenclature**

If the fused ring system cannot be named on the basis of normal fusion nomenclature, or the use of replacement nomenclature with the corresponding hydrocarbon, or even when using a less preferred parent component, then it is treated as a bridged fused system (see FR-8). The fused ring portion should be selected using FR-8.2.

Examples:



1,12-ethenobenzo[4,5]cyclohepta[1,2,3-*de*]naphthalene
not 1,12-ethenobenzo[*c*]phenanthrene
(preferred fused ring system, see FR-8.2.d; 7,6,6,6 rings preferred to 6,6,6,6 rings)



8,7-(azenoetheno)cyclohepta[4,5]cycloocta[1,2-*b*]pyridine
not 6,7-buta[1,3]dienocycloocta[1,2-*b*:5,6-*c*']dipyridine
(maximum number of atoms in fused ring system, see FR-8.2.b)
CAS name 8,7-(nitriloetheno)cyclohepta[4,5]cycloocta[1,2-*b*]pyridine
Beilstein name 8,7-epi[1]azaprop-2-en-3-yl-1-ylidene-cyclohepta[4,5]cycloocta[1,2-*b*]pyridine

FR-8 Bridged Fused Ring Systems

FR-8.1 Procedure for naming bridged systems

This section provides an outline of the procedure for naming bridged polycyclic fused ring parent hydrides.

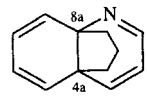
FR-8.1.1 *Selection of bridge*

If a polycyclic skeleton cannot be completely named as a fused ring system then possible ways of naming the skeleton as a bridged fused ring system are considered. The bridge is selected as described in FR-8.2 to give the preferred fused ring system.

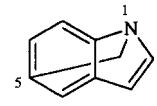
FR-8.1.2 *Naming of ortho- or ortho- and peri-fused portion*

The skeleton of the portion of the structure which remains after removal of the bridge(s) is named following FR-4. Note that the maximum number of non-cumulative double bonds is assigned after insertion of the bridge. Hence in order to allow for the necessary free valencies to the bridge the fused ring system may differ from the isolated fused ring system in the number of non-cumulative double bonds (see FR-9.1) and/or the need for indicated hydrogen (see FR-9.3). If needed indicated hydrogen is used to identify the required isomer (see FR-9).

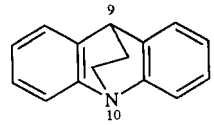
Examples:



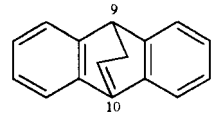
4a,8a-propanoquinoline



1,5-methanoindole
CAS name 1,5-methano-1*H*-indole



9*H*-9,10-ethanoacridine



9*H*-9,10-(ethanylylidene)anthracene
Beilstein name 9*H*-9,10-epiethanylylidene-anthracene

FR-8.1.3 *Order of citation of bridges*

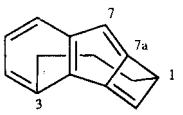
Bridges are cited by the technique described in FR-8.4. If there is more than one independent bridge they are cited in alphabetical order (see FR-8.4.1) unless identical (see FR-8.4.4). Dependent bridges are cited in front of all independent bridges. If there is a choice of attachment locants see FR-8.4.3.

FR-8.2 **Selection of fused ring system to be bridged**

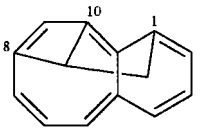
The bridge (or bridges) is selected which results in the preferred fused ring system remaining by the following criteria applied in order. For the following examples see Note 3 to FR-1.4 on double bonds.

a. The fused ring system before bridging containing the maximum number of rings.

Example:



not



1*H*-1,3-propanocyclobuta[*a*]indene
(fused ring system has 3 rings)

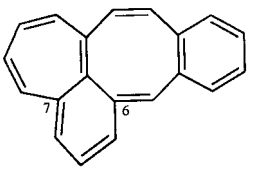
8,10,1-(ethane[1,1,2]triyl)benzo[8]annulene
(fused ring system has 2 rings)

Beilstein name 6,7,8,9-tetrahydro-1,9-cyclo-cycloocta[*cd*]indene

Note Both structures have the same carbon skeleton although different numbers of double bonds.

b. The fused ring system including the maximum number of skeletal atoms.

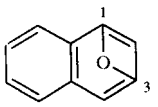
Example:



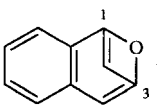
6,7-(prop[1]en[1]yl[3]ylidene)benzo[*a*]cyclohepta[*e*][8]annulene
not 7,6-(prop[1]en[1]yl[3]ylidene)benzo[*a*]cyclohepta[*e*][8]annulene (moves double bonds)
nor 4,5-buta[1,3]dienodibenzo[*a*,*d*][8]annulene
nor 6,10,15-(methanediylylidene)benzo[15]annulene (criterion a)

c. The arrangement having the minimum number of heteroatoms in the fused ring system.

Example:



not



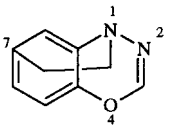
1,3-epoxynaphthalene

1,3-(metheno)isochromene

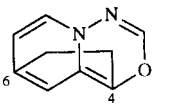
Note *CAS* and *Beilstein* prefer the heteroatoms in the fused ring portion. Hence they call this example 1,3-metheno-1*H*-2-benzopyran and 1,3-methenoisochromene respectively.

d. The most preferred fused ring system, according to FR-2.3 applied to the whole fused ring system.

Examples:

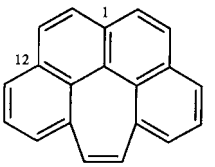


not

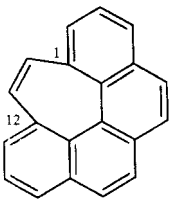


1,7-ethano[4,1,2]benzoxadiazine

4,6-ethanopyrido[1,2-*d*][1,3,4]oxadiazine
(1,2,4 preferred to 1,3,9, see FR-2.3.h)



not

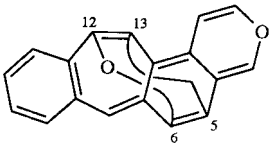


1,12-ethenobenzo[4,5]cyclohepta[1,2,3-*de*]naphthalene (7,6,6,6 rings preferred 6,6,6,6 rings, see FR-2.3.c)

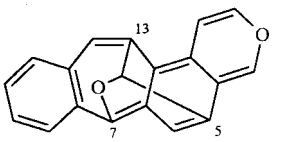
1,12-ethenobenzo[*c*]phenanthrene

e. The number of composite bridges being minimised.

Example:



not

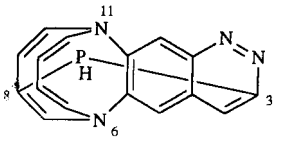


6,12-epoxy-5,13-methanobenzo[4,5]-cyclohepta[1,2-*f*]isochromene

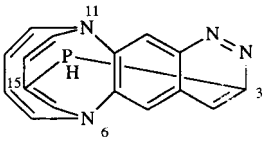
7,5,13-(epoxymethanetriyl)benzo[4,5]-cyclohepta[1,2-*f*]isochromene

f. The number of dependent bridges being a minimum.

Example:



not

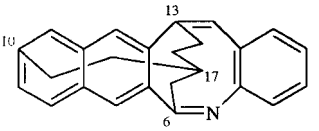


6,11-buta[1,3]dieno-3,8-phosphano-[1,4]diazocino[2,3-*g*]cinnoline

3,15-phosphano-6,11-buta[1,3]dieno-[1,4]diazocino[2,3-*g*]cinnoline

g. The number of atoms in dependent bridges being a minimum.

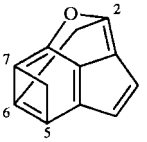
Example:



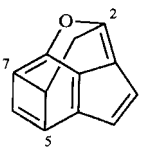
6,17-methano-10,13-pentanonaphtho[2,3-*c*][1]benzazocine
not 13,17-ethano-6,10-butanonaphtho[2,3-*c*][1]benzazocine
nor 10,17-ethano-6,13-butanonaphtho[2,3-*c*][1]benzazocine

h. The number of bivalent bridges (see FR-1.4.3) being a maximum. Similarly '-ylylidene' is preferred as a trivalent bridge to '-triyl' etc. (*i.e.* '-diyl' is preferred to '-ylylidene', '-triyl', '-diylidene', '-diylylidene' or '-tetrayl', *etc.*).

Examples:

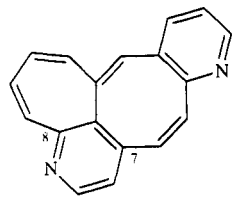


not

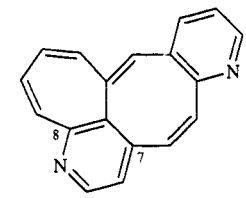


2,6:5,7-dimethanoindeno[7,1-*bc*]furan

5,7,2-(ethane[1,1,2]triyl)indeno[7,1-*bc*]furan



not

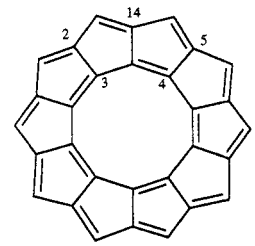


8,7-(azenoetheno)cyclohepta[4,5]-cycloocta[1,2-*b*]pyridine

8,7-(azenoethanediylidene)cyclohepta[4,5]-cycloocta[1,2-*b*]pyridine

i. The location of bridges which results in the preferred attachment locants firstly for independent bridges then dependent bridges.

Example:

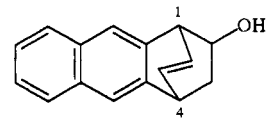


5,14-(metheno)-2,3,4-(prop[2]en[1,3]diyl[1]ylidene)dicyclopenta[*f,f'*]pentaleno[1,2-*a*:6,5-*a'*]dipentalene
not 5,14-(metheno)-2,4,3-(prop[2]en[1,3]diyl[1]ylidene)dicyclopenta[*f,f'*]pentaleno-[1,2-*a*:6,5-*a'*]dipentalene
See also FR-1.4 Note 2.

Note This ring system appears to have a ring in the middle which is not named. The ten-membered ring is created by the bridges on the fully specified fused ring system.

j. The fused ring system which gives the lowest locant(s) for the principal characteristic group.

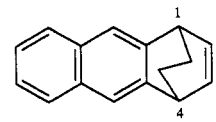
Example:



1,2,3,4-tetrahydro-1,4-ethenoanthracen-2-ol
not 1,4-dihydro-1,4-ethanoanthracen-11-ol

k. The fused ring system being chosen which includes the maximum number of non-cumulative double bonds.

Example:



1,4-dihydro-1,4-ethanoanthracene
not 1,2,3,4-tetrahydro-1,4-ethenoanthracene

FR-8.3 **Naming bridges**

FR-8.3.1 *Simple bivalent bridges*

a. An acyclic bivalent hydrocarbon bridge is named as a prefix derived from the corresponding hydrocarbon name by changing the final 'e' to 'o'. The locant of a double bond, if present, is indicated in square brackets between the hydrocarbon prefix and the ending '-eno'. If there is a choice low numbers are preferred (*e.g.* prop[1]eno rather than prop[2]eno). Note that this is not the locant used in the final numbering of the bridged fused ring system (see FR-8.5).

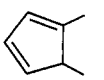
Examples:

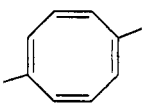
methano	$-CH_2-$	
ethano	$-CH_2CH_2-$	
propano	$-CH_2CH_2CH_2-$	
butano	$-CH_2CH_2CH_2CH_2-$	
etheno	$-CH=CH-$	
prop[1]eno	$-CH=CHCH_2-$	*CAS* and *Beilstein* use propeno
but[1]eno	$-CH=CHCH_2CH_2-$	Formerly [1]buteno which is still used by *CAS*; *Beilstein* uses but-1-eno
but[2]eno	$-CH_2CH=CHCH_2-$	Formerly [2]buteno which is still used by *CAS*; *Beilstein* uses but-2-eno
buta[1,3]dieno	$-CH=CHCH=CH-$	Formerly [1,3]butadieno which is still used by *CAS*; *Beilstein* uses buta-1,3-dieno

b. A monocyclic hydrocarbon bridge other than benzene is named by the same prefix as that used as a fusion prefix (FR-2.1.1). To distinguish between the two the prefix for a bridge has 'epi-' added in front of the name. The bridge is assumed to have the maximum number of non-cumulative double bonds consistent with the attachments to the fused ring system or to other bridges. The positions of the free valencies are indicated by the relevant locants in square brackets directly in front of the bridge name. Note that these locants are not those assigned to the final structure (see FR-8.6).

Examples:

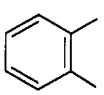
epicyclopropa  Indicated hydrogen is needed to locate double bonds (see FR-9.3.2). *Note* [1,2] is implied but not stated. *CAS* uses *endo*-cyclopropa, *Beilstein* uses [1,2]cycloprop-2-eno

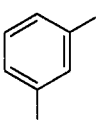
[1,2]epicyclopenta  Indicated hydrogen is needed to locate double bond (see FR-9.3.2). *CAS* uses [1',2']-*endo*-cyclopenta, *Beilstein* uses [1,2]cyclopenta[2,4]dieno

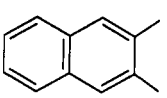
[1,5]epicycloocta  *CAS* uses [1',5']-*endo*-cycloocta, *Beilstein* uses [1,5]cycloocta-1,3,5,7-tetraeno

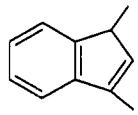
c. Any other cyclic hydrocarbon is named as a prefix derived from the corresponding unsaturated hydrocarbon name in Appendix 1 by replacing the terminal '-e' by '-o'. If the name of the bridge is the same as the fusion prefix the bridge is indicated by adding 'epi-' in front of the name. The 'i' is elided if followed by a vowel. Locants are used in the same way as in section b.

Examples:

[1,2]benzeno  Formerly *o*-benzeno which is used by *Beilstein*.*CAS* uses [1',2']-benzeno

[1,3]benzeno  Formerly *m*-benzeno which is used by *Beilstein*; *CAS* uses [1',3']-benzeno

[2,3]naphthaleno  *CAS* uses [2',3']-naphthaleno

[1,3]epindeno 

Indicated hydrogen is needed to locate the double bonds (see FR-9.3.2). *CAS* uses [1',3']-*endo*-indeno, Beilstein uses [1,3]-epiindeno

d. An acyclic heteroatom bridge is named by the appropriate prefix. Non-standard valence states are given using the λ-convention (ref 17).

Examples:

epoxy	-O-	*Beilstein* uses epioxido
epidioxy	-OO-	*Beilstein* uses epidioxido
epitrioxy	-OOO-	*Beilstein* uses epitrioxido
epithio	-S-	*Beilstein* uses episulfano
λ^4-sulfano	$-SH_2-$	*Beilstein* uses epi-λ^4-sulfano
λ^6 -sulfano	$-SH_4-$	
epidithio	-SS-	*Beilstein* uses epidisulfano
episeleno	-Se-	*Beilstein* uses episelano
epitelluro	-Te-	*Beilstein* uses epitellano
epimino	-NH-	formerly imino which is still used by *CAS*; *Beilstein* uses epiazano
diazano	-NHNH-	formerly biimino which is still used by *CAS*; *Beilstein* uses epidiazano
diazeno	-N=N-	formerly azo which is still used by *CAS*; *Beilstein* uses epidiazeno
triaz[1]eno	-N=NNH-	formerly azimino which is still used by *CAS*; *Beilstein* uses epitriazeno or for -N=N-NR- epitriaz-1-eno
phosphano	-PH-	*CAS* uses phosphinidene; *Beilstein* uses epiphosphano
arsano	-AsH-	*CAS* uses arsinidene; *Beilstein* uses epiarsano
stibano	-SbH-	*CAS* uses stibylene; *Beilstein* uses epistibano
silano	$-SiH_2-$	*Beilstein* uses episilano
germano	$-GeH_2-$	*Beilstein* uses epigermano
stannano	$-SnH_2-$	
borano	-BH-	*CAS* uses borylene; *Beilstein* uses epiborano

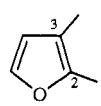
Note *CAS* names hydrocarbons and non-nitrogenous heterocyclic systems with epimino bridges by use of the suffix -imine preceded by the appropriate locants and with elision of a final 'e' if present *e.g.* naphthalen-1,4-imine.

e. A heterocyclic bridge is named as a prefix derived from the corresponding heterocyclic compound listed in Appendix 2 by adding an 'o' with elision of a final 'e' if present. If the heterocyclic system requires the citation of locants these are given in square brackets in front of the name. If the name of the bridge is the same as the fusion prefix the bridge is indicated by adding 'epi-' in front of the name. The 'i' is elided if followed by a vowel.

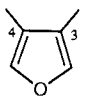
Examples:

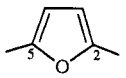
epoxireno 

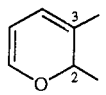
CAS uses *endo*-oxireno, and *endo*-oxirano for dihydroepoxireno; *Beilstein* uses etheno and ethano with epoxy substituent prefixes.

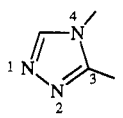
[2,3]furano 

CAS uses [2',3']-furano

[3,4]furano  *CAS* uses [3',4']-furano

[2,5]furano  *CAS* uses [2',5']-furano

[2,3]epipyrano  Indicated hydrogen is needed to locate the double bond see (FR-9.3.2). *CAS* uses [2',3']-*endo*-pyrano

[3,4]epi[1,2,4]triazolo  *CAS* uses [3',4']-*endo*-[1,2,4]triazolo

FR-8.3.2 *Simple polyvalent bridges*

Polyvalent bridges are cited within round brackets.

Note Brackets are not used by *CAS* or *Beilstein*.

a. A polyvalent bridge consisting of one atom (other than hydrogen) is named by the appropriate prefix.

Examples:

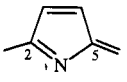
(metheno)	–CH=	*CAS* and *Beilstein* use metheno without brackets
(methanetriyl)		*CAS* uses metheno; *Beilstein* uses epimethanetriyl
(methanediylylidene)		*CAS* uses methyno; *Beilstein* uses epimethanediylylidene
(methanetetrayl)		*CAS* uses methyno; *Beilstein* uses epimethanetetrayl
(azeno)	–N=	*CAS* uses nitrilo; *Beilstein* uses epiazanylylidene
(azanetriyl)		*CAS* uses nitrilo; *Beilstein* uses epiazanetriyl
(phospheno)	–P=	*CAS* uses phosphinidyne; *Beilstein* uses epiphosphanylylidene
(phosphanetriyl)		*CAS* uses phosphinidyne; *Beilstein* uses epiphosphanetriyl

b. A polyvalent polyatomic bridge is named as the appropriate polyvalent group (see A-4.4, 4.5 in ref 3 and R-2.5, R-3.1.4 in ref 3a). If necessary the positions of the free valencies are indicated by the appropriate locants directly in front of the associated ending. The ending '-ylidene' is restricted to those cases where there is a double bond between the bridge and the fused ring system. If there is a choice of numbering of the bridge preference is given to low numbers for (a) -yl, (b) -ylidene, (c) double bonds.

Note The previous edition of these rules (ref 3) also used '-ylidene' to indicate bonds to two different positions (and '-ylidyne' to indicate bonds to three positions) and cited the locant(s) nearest to the hydrocarbon or numerical prefix in front of that prefix. This practice is still used by *CAS*.

Examples:

(ethanylylidene)	$-CH_2CH=$	*Beilstein* uses epiethanylylidene
(ethane[1,1,2]triyl)		*CAS* uses ethanylylidene; *Beilstein* uses epiethane-1,1,2-triyl
(ethanediylidene)	=CHCH=	*Beilstein* uses epiethanediylidene

(ethane[1,1]diyl[2]ylidene)	$-\overset{\vert}{C}HCH=$	*Beilstein* uses epiethane-1,1-diyl-2-ylidene
(ethane[1,1,1,2]tetrayl)	$-\overset{\vert}{C}CH_2-$	*CAS* uses ethanylylidyne
(ethane[1,1,2,2]tetrayl)	$-\overset{\vert}{C}H\overset{\vert}{C}H-$	*CAS* uses ethanediylidene; *Beilstein* uses epiethane-1,1,2,2-tetrayl
(ethene[1,1,2]triyl)	$-\overset{\vert}{C}=CH-$	*CAS* uses ethenylylidene
(propane[1,2,3]triyl)	$-CH_2\overset{\vert}{C}HCH_2-$	
(propan[1]yl[3]ylidene)	$-CH_2CH_2CH=$	
(propane[1,1,3]triyl)	$-\overset{\vert}{C}HCH_2CH_2-$	*CAS* uses [1]propanyl[3]ylidene
(propane[1,2]diyl[3]ylidene)	$-CH_2\overset{\vert}{C}HCH=$	
(propane[1,1,2,3]tetrayl)	$-\overset{\vert}{C}H\overset{\vert}{C}HCH_2-$	*CAS* uses [1,2]propanediyl[3]ylidene
(propane[1,1,1,3]tetrayl)	$-\overset{\vert}{C}CH_2CH_2-$	*CAS* uses [1]propanyl[3]ylidyne
(prop[1]en[1]yl[3]ylidene)	$-CH=CHCH=$	
(prop[2]ene[1,1,3]triyl)	$-\overset{\vert}{C}HCH=CH-$	*CAS* uses [1]propen[1]yl[3]ylidene
(prop[2]ene[1,3]diyl[1]ylidene)	$=\overset{\vert}{C}CH=CH-$	*CAS* uses [1]propen[1]yl[3]ylidyne
(propan[1]yl[2,3]diylidene)	$-CH_2\overset{\Vert}{C}CH=$	
(propan[2]yl[1,3]diylidene)	$=CH\overset{\vert}{C}HCH=$	
(propane[1,1,3]triyl[2]ylidene)	$-\overset{\vert}{C}HC\overset{\Vert}{C}CH_2-$	
(propane[1,2,2]triyl[3]ylidene)	$-CH_2\overset{\vert}{C}CH=$	
(propane[1,1,2,2,3]pentayl)	$-\overset{\vert}{C}H\overset{\vert}{C}\overset{\vert}{C}CH_2-$	*CAS* uses [1]propanyl[2,3]diylidene
(buta[1,3]diene[1,1,4]triyl)	$-\overset{\vert}{C}H=CHCH=CH-$	*CAS* uses [1,3]butadien[1]yl[4]ylidene
(but[1]ene[1,3]diyl[4]ylidene)	$-CH=CH\overset{\vert}{C}HCH=$	
(but[3]ene[1,1,2,4]tetrayl)	$-\overset{\vert}{C}H\overset{\vert}{C}HCH=CH-$	
(diazanediylidene)	$=N-N=$	formerly azino which is still used by *CAS*; *Beilstein* uses epidiazanediylidene
(pyrrol[2]yl[5]ylidene)		*CAS* uses [2]pyrrolyl[5]ylidene; *Beilstein* uses epipyrrol-2-yl-5-ylidene

FR-8.3.3 *Composite bridges*

Composite bridges are named by combining the names of two or more simple bridge prefixes. However see FR-8.5 for a different treatment when the fused ring system is named using replacement nomenclature. Unless cited first ep(i) is omitted. The prefixes are cited without elision in order starting from the preferred terminal prefix based on the following criteria applied in turn until a decision is reached:

a. The simple bridge containing the preferred heteroatom [see table 1 (ref 9)].

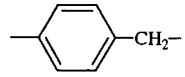
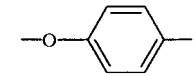
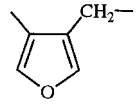
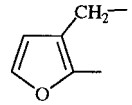
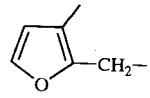
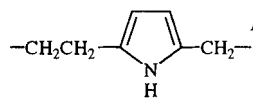
b. The simple bridge containing the preferred ring system (see FR-2.3).

c. The simple bridge containing the longer acyclic chain.

d. The simple bridge which occurs first alphabetically.

Composite bridges are cited within round brackets. Locants associated with a cyclic bridge component are cited in attachment order. If an acyclic bridge component requires internal numbering it is numbered in the direction implied by the bridge name (*cf.* numbering in FR-8.3.1.a). Acyclic bridge components in a composite bridge are only attached to other components through terminal positions *e.g.* only 1 and 3 of propane-1,2,3-triyl. If polyvalent acyclic bridge components are used care must be taken to check that there is no ambiguity. If there is ambiguity then alternative arrangements such as a dependent bridge must be considered.

Examples:

(epoxymethano)	$-OCH_2-$	*Beilstein* uses oxaethano
(epiminoethano)	$-NHCH_2CH_2-$	formerly iminoethano which is still used by *CAS*; *Beilstein* uses [1]azapropano
(epoxyethane[1,1,2]triyl)	$-O\overset{|}{C}HCH_2-$	*CAS* uses (epoxy[2]ethanyl[1]ylidene) *Beilstein* uses epi[1]oxapropane-1,2,3-triyl
(epoxyethane[1,2,2]triyl)	$-OCH_2\overset{|}{C}H-$	*CAS* uses (epoxyethanylylidene); *Beilstein* uses epi[1]oxapropane-1,3,3-triyl
(epoxyprop[1]eno)	$-OCH{=}CHCH_2-$	
(epoxyprop[2]eno)	$-OCH_2CH{=}CH-$	*CAS* uses (epoxy[2]propeno); *Beilstein* uses [1]oxabut-3-eno
([1,4]benzenomethano)		*Beilstein* prefers cyclophane name here
(epoxy[1,4]benzeno)		*Beilstein* prefers cyclophane name here
(ethanoiminomethano)	$-CH_2CH_2NHCH_2-$	*CAS* uses (ethaniminomethano); *Beilstein* uses [2]azabutano
(methanooxymetheno)	$-CH_2OCH{=}$	*CAS* uses (methanoxymetheno); *Beilstein* uses epi[2]oxapropan-1-yl-3-ylidene
(methanetriyloxymethano)	$-\overset{|}{C}HOCH_2-$	*CAS* uses (methanoxymetheno) for this also; *Beilstein* uses epi[2]oxapropane-1,1,3-triyl
(epoxymethanoazenometheno)	$-OCH_2N{=}CH-$	*CAS* uses (epoxymethanonitrilometheno); *Beilstein* uses [1]oxa[3]azabut-3-eno
(epoxymethenoazenomethano)	$-O-CH{=}N-CH_2-$	*CAS* uses (epoxymethenonitrilomethano); *Beilstein* uses [1]oxa[3]azabut-2-eno
([3,4]furanomethano)		*Beilstein* prefers a cyclophane name
([2,3]furanomethano)		*Beilstein* prefers a cyclophane name
([3,2]furanomethano)		*Beilstein* prefers a cyclophane name
(ethano[2,5]pyrrolomethano)		*Beilstein* prefers a cyclophane name

FR-8.3.4 *Elision*

Vowels are not elided for bridges.

CAS elides the terminal 'a' of a monocyclic hydrocarbon bridge when followed by a vowel. With composite bridges the terminal 'o' of benzeno or an acyclic component is elided when followed by a component of the composite bridge which starts with a vowel (iminoethano is an exception). In all other cases a terminal 'a', 'e', or 'o' is not elided. Examples of *CAS* index names are:

11*H*-9,10[1',2']-*endo*-cyclopentanthracene
9,10-(methaniminomethano)anthracene
6,13-(imino[1,2]benzenimino)dibenzo[*d*,*i*][1,3,6,8,2,7]tetrazadiphosphecine

FR-8.4 Naming of bridged fused ring systems

FR-8.4.1 *Order of citation of bridges*

If there is more than one bridge they are cited in alphabetical order unless one is dependent on another (see FR-8.7.a). In this case the dependent bridge is cited in front of all independent bridges. Identical bridges of the same order are quoted using the appropriate multiplicative prefix (see FR-8.4.4).

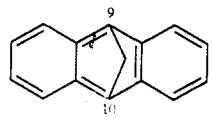
FR-8.4.2 *Attachment locants*

The fused ring system is numbered in the usual way (see FR-5).

a. Symmetric bridges

The locants of the positions on the fused ring system to which the bridge is attached are cited in numerical order in front of the bridge.

Example:

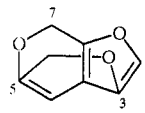


9,10-methanoanthracene

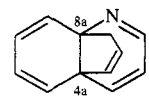
b. Asymmetric bridges

The locants of the positions on the fused ring system to which the bridge is attached are cited in the order implied by the name of the asymmetric bridge (locant order for the free valencies of the bridge is given by FR-8.3). If there is a choice, locants are cited in numerical order. See FR-9.3.2 for the use of indicated hydrogen.

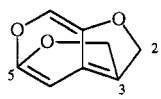
Examples:



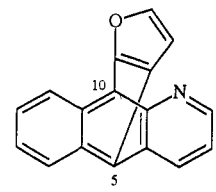
7*H*-3,5-(epoxymethano)furo[2,3-*c*]pyran



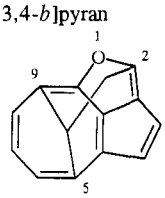
4a,8a-prop[1]enoquinoline



2*H*-5,3-(epoxymethano)furo[2,3-*c*]pyran
Beilstein name 2*H*-5,3-oxaethano-furo[3,4-*b*]pyran



10,5-[2,3]furanobenzo[*g*]quinoline



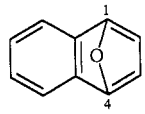
1-oxa-5,9,2-(ethane[1,1,2]triyl)cycloocta[1,2,3-*cd*]pentalene

FR-8.4.3 *Choice of attachment locants*

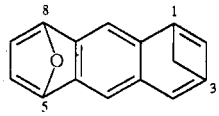
If there is a choice of attachment locants after the application of FR-8.4.2 preference is given in the following order:

a. The lowest set of locants for all the bridge attachment points considered as a set.

Examples:



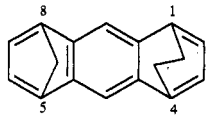
1,4-epoxynaphthalene
not 5,8-epoxynaphthalene



5,8-epoxy-1,3-methanoanthracene
not 1,4-epoxy-5,7-methanoanthracene (1,3,5,8 preferred to 1,4,5,7)

b. Lowest locants in the order of citation for the bridges.

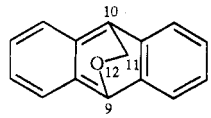
Example:



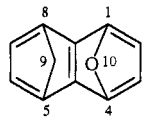
1,4-ethano-5,8-methanoanthracene

Note *CAS* and *Beilstein* select when there is a choice of attachment locants those which result in lower numbers for heteroatoms in preference to the above criterion. (See FR-8.6 for numbering of bridge atoms.)

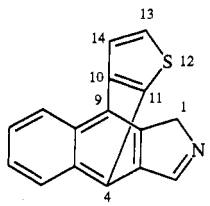
Examples:



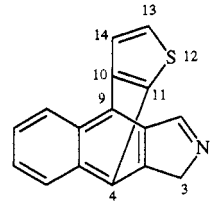
9,10-(epoxymethano)anthracene
CAS name 10,9-(epoxymethano)anthracene and
Beilstein name 10,9-oxaethano-anthracene (hence oxygen is atom 11 not 12)



1,4-epoxy-5,8-methanonaphthalene
CAS name 5,8-epoxy-1,4-methanonaphthalene
Beilstein name 5,8-epioxido-1,4-methano-naphthalene



1*H*-4,9-[2,3]thiophenobenzo[*f*]isoindole
CAS name 4,9[2',3']-thiopheno-1*H*-benz[*f*]isoindole



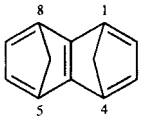
3*H*-4,9-[2,3]thiophenobenzo[*f*]isoindole
CAS name 4,9[3',2']-thiopheno-1*H*-benz[*f*]isoindole

Note See FR-9.3.2 for the use of indicated hydrogen and FR-8.6 for numbering of bridge atoms.

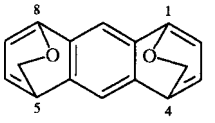
FR-8.4.4 *Treatment of identical bridges*

When there are two or more identical bridges this is indicated by the use of di-, tri-, *etc.* with single bridges (or bis-, tris- *etc.* with composite bridges or if di-, tri-, *etc.* would be ambiguous). The locants of the bridges are separated by a colon.

Examples:

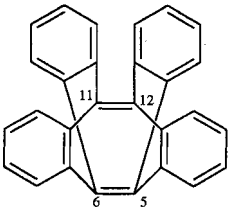


1,4:5,8-dimethanonaphthalene



1,4:8,5-bis(epoxymethano)anthracene

Beilstein name 1,4;8,5-bis-oxaethano-anthracene



5,12:6,11-di[1,2]benzenodibenzo[*a*,*e*][8]annulene

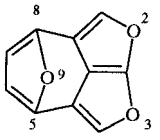
CAS name 5,12[1',2']:6,11[1",2"]-dibenzenodibenzo[*a*,*e*]cyclooctene

Beilstein name 5,12:6,11-di-*o*-benzeno-dibenzo[*a*,*e*]cyclooctene

FR-8.5 **Bridged fused ring systems where replacement nomenclature is used**

If the fused ring system can only be named using replacement nomenclature (see FR-7.1) any heteroatoms in a bridge are also named using replacement nomenclature. The replacement terms are cited in front of the name of the corresponding hydrocarbon bridged fused ring system.

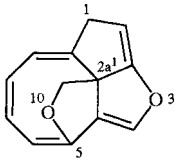
Examples:



2,3,9-trioxa-5,8-methanocyclopenta[*cd*]azulene

CAS name 5,8-epoxy-2,3-dioxacyclopent[*cd*]azulene

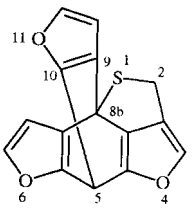
Beilstein name 2,3-dioxa-5,8-epioxido-cyclopent[*cd*]azulene



1*H*-3,10-dioxa-2a^1,5-ethanocycloocta[*cd*]pentalene

CAS name 4*H*-9,9b-(epoxymethano)-2-oxacycloocta[*cd*]pentalene

Beilstein name 8*H*-3,12-cyclo-furo[3',2':1,5]cyclopenta[1,2-*c*]oxonine



2*H*,5*H*-4,6,11-trioxa-1-thia-5,8b-[1,2]epicyclopentacyclopenta[*cd*]-*s*-indacene

CAS name 2*H*,5*H*-5,8b[2',3']-furano-4,6-dioxa-1-thiacyclopent[*cd*]-*s*-indacene

Beilstein name 2*H*,5*H*-4,6-dioxa-1-thia-5,8b-[2,3]furano-cyclopent[*cd*]-*s*-indacene

Note *CAS* and *Beilstein* use the appropriate bridge name which includes the heteroatom when replacement prefixes are needed to name the fused ring system. *CAS* cites the bridge prefixes before replacement prefixes, whereas *Beilstein* cites replacement prefixes before bridge prefixes.

FR-8.6 **Numbering of bridge atoms**

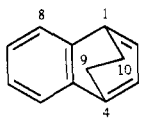
Bridge atoms are numbered continuing from the highest locant of the fused ring system. If there is more than one bridge atom (excluding hydrogen) the numbering starts at the chain end or ring atom connected to the bridgehead possessing the highest number. With a composite bridge each component of the composite bridge is completely numbered before the next component. If there is a choice of numbers then preference is given in the following order to:

a. low locants for heteroatoms

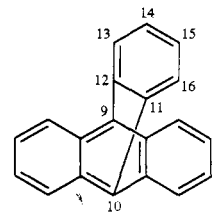
b. low locants for bridgehead atoms within a bridge

c. the remaining atoms (excluding hydrogen) being numbered continuously

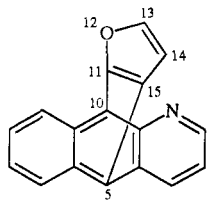
Examples:



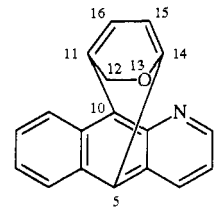
1,4-ethanonaphthalene



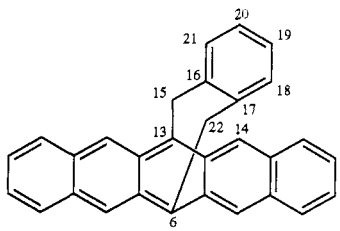
9,10-[1,2]benzenoanthracene



10,5-[2,3]furanobenzo[*g*]quinoline

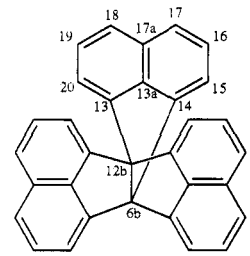


12*H*-5,10-[2,5]epipyranobenzo[*g*]quinoline



6,13-(methano[1,2]benzenomethano)pentacene

Beilstein name 1(1,2)-benzena-3(6,13)-pentacena-cyclobutaphane

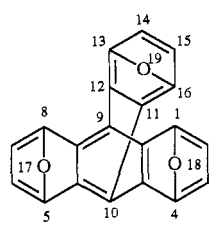


6b,12b-[1,8]naphthalenoacenaphthyleno-[1,2-*a*]acenaphthylene

FR-8.7 **Order of numbering bridges**

a. Independent bridges are numbered before dependent bridges.

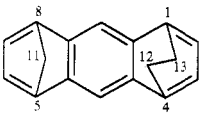
Example:



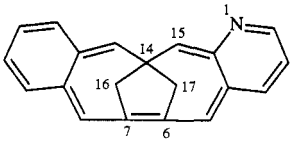
13,16-epoxy-1,4:5,8-diepoxy-9,10-[1,2]benzenoanthracene
(13,16-epoxy is a dependant bridge)

b. If there is more than one bridge of the same order preference is given to the bridge attached to the bridgehead with the higher locant at the first point of difference.

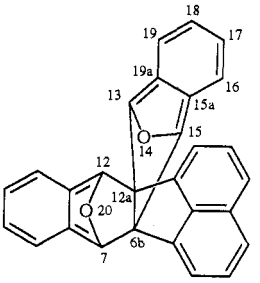
Examples:



1,4-ethano-5,8-methanoanthracene



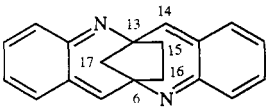
6,14:7,14-dimethanobenzo[7,8]cycloundeca[1,2-*b*]pyridine



6b,12a-([1,3][2]benzofurano)-7,12-epoxybenzo[*k*]fluoranthene

c. If two bridges are attached to the same bridgehead atoms they are numbered in alphabetical order.

Examples:



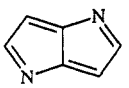
6,13-ethano-6,13-methanodibenzo[*b*,*g*][1,6]diazecine

FR-9 Indicated Hydrogen

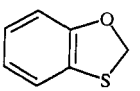
FR-9.1 Maximum number of non-cumulative double bonds

The names of polycyclic fused ring systems are considered to correspond to the compound with the maximum number of non-cumulative double bonds consistent with the appropriate valency of the skeletal atoms.

Examples:



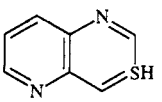
pyrrolo[3,2-*b*]pyrrole



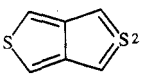
2*H*-1,3-benzoxathiole
2*H* may be omitted

If non-standard valence states are present this must be indicated using the λ-convention (ref 17) [and if necessary the δ-convention (ref 19)]. The corresponding valency is used in assigning the non-cumulative double bonds.

Examples:



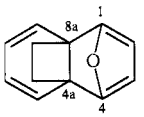
3λ^4-pyrido[3,2-*d*][1,3]thiazine



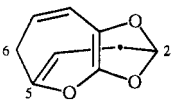
2λ^{4}δ^2-thieno[3,4-*c*]thiophene

With bridged systems the assignment of non-cumulative double bonds to the parent fused ring system is applied after allowance for the bonds existing between the bridge(s) and the fused ring system. Rings which form part of a bridge are treated separately, after consideration of free valencies implied by the name.

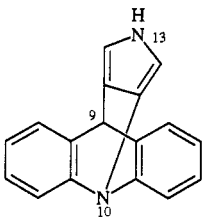
Examples:



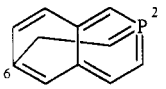
1,4-epoxy-4a,8a-ethanonaphthalene



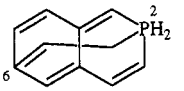
2*H*,6*H*-2,5-(ethanylylidene)[1,3]dioxolo[4,5-*b*]oxepine



9*H*,13*H*-9,10-[3,4]epipyrroloacridine



2$\lambda^5$2δ^2-6,2-(ethanylylidene)isophosphinoline

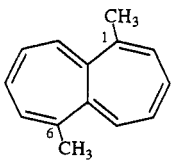


2*H*-2λ^5-2,6-(ethanylylidene)isophosphinoline

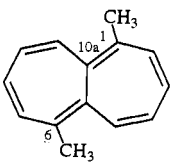
FR-9.2 **Localised double bonds**

If it is necessary to identify isomers which differ only by virtue of the location of localised double bonds this is indicated by the use of the Greek letter Δ. The locant(s) cited correspond to the lowest numbered atom of a localised double bond.

Examples:



1,6-dimethyl-Δ^1-heptalene



1,6-dimethyl-$\Delta^{1(10a)}$-heptalene

FR-9.3 **Citation of indicated hydrogen**

When a name applies equally to two or more isomeric 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 an italic *H* for each of these hydrogen atoms. These atoms are called indicated hydrogen.

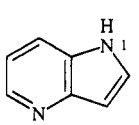
Notes 1. Indicated hydrogen is often omitted for the normally encountered isomer of some ring systems (see rule B-2.11 ref 3, and note a to Table 20 and 23 ref 3a) *i.e.* carbazole, fluorene, imidazole, indazole, indene, indole, isochromene, isoindole, perimidine, phenalene, phenothiazine, phenoxazine, purine, pyrazole, pyrrole, selenoxanthene, telluroxanthene, thioxanthene, xanthene.

2. Indicated hydrogen may be omitted where there is no ambiguity. For example at a position located between two divalent atoms (see example 2 under FR-9.1).

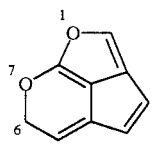
FR-9.3.1 *Ortho- or ortho- and peri-fused ring systems*

If indicated hydrogen is needed it is identified by the locant of the relevant position (see FR-5) cited in front of the name of the whole ring system, including replacement terms, if used.

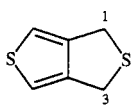
Examples:



1*H*-pyrrolo[3,2-*b*]pyridine



6*H*-1,7-dioxacyclopenta[*cd*]indene

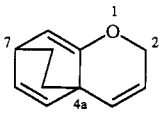


1*H*,3*H*-thieno[3,4-*c*]thiophene

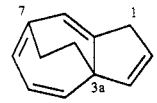
FR-9.3.2 *Bridged systems*

If indicated hydrogen is necessary to distinguish between isomers of the fused ring system and/or of the bridge indicated hydrogen is cited in front of the name.

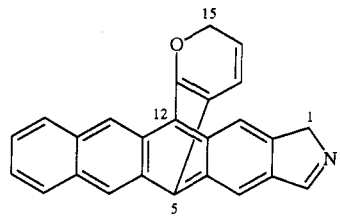
Examples:



2*H*,7*H*-4a,7-ethanochromene
CAS name 7*H*-4a,7-ethano-2*H*-1-benzopyran



1*H*-3a,7-ethanoazulene



1*H*,15*H*-12,5-[2,3]epipyranoanthra[2,3-*f*]isoindole
CAS name 15*H*-12,5[2',3']-*endo*-pyrano-1*H*-anthra[2,3-*f*]isoindole

The previous edition of these rules (ref 3) separated the indicated hydrogen needed for a bridge from that used for the fused ring system (see A-34.4 for example). This system is still used by *CAS*, who would also use it in, for example, 3a,6-ethano-3a*H*-indene but not with the bridge [2]pyrrolyl[5]ylidene (*cf.* rule B-5.12).

FR-9.4 **Partially hydrogenated fused ring sysem**

Certain partially hydrogenated fused ring systems are named separately (see Table 21 and 24 of ref 3a). These should not be used as components in fusion nomenclature. The following names are retained: chromane, indane, indoline, isochromane, isoindoline, selenochromane, selenoisochromane, tellurochromane, telluroisochromane, thiochromane, thioisochromane. In the previous edition of these rules (see rule A-23.1, ref 3) several other examples were listed *i.e.* acenaphthene, cholanthrene, aceanthrene, acephenanthrene, violanthrene, isoviolanthrene. These are no longer recommended. *Beilstein* uses all of these except indoline, isoindoline, violanthrene and isoviolanthrene. None are used by *CAS*. The system for naming partially hydrogenated hydrocarbon fused ring systems in rule A-23.5 (ref 3) is abandoned.

References

1. A.M. Patterson and C.E. Curran, A system of organic nomenclature, *J. Am. Chem. Soc.* **39**, 1623-1638 (1917).

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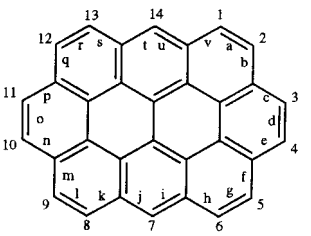
Appendix 1

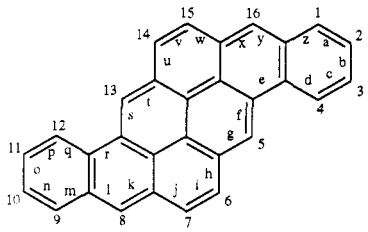
Hydrocarbon parent components in order of decreasing seniority.

1	Polyphenylene	$(C_6)_m.C_{2m}$	*cf.* 33 ($m > 8$)	(see FR-2.1.5)
2	Polynaphthylene	$(C_6)_{2k}.C_{2k}$	*cf.* 25 ($k > 4$)	(see FR-2.1.6)
3	Polyacene	$(C_6)_n$	*cf.* 40 ($n > 9$)	(see FR-2.1.2)
4	Polyaphene	$(C_6)_n$	*cf.* 31 or 35 ($n > 9$)	(see FR-2.1.3)
5	Polyhelicene	$(C_6)_n$	*cf.* 32 ($n > 9$)	(see FR-2.1.7) *Note* a
6	Nonaphenylene	$(C_6)_9.C_{18}$	*cf.* 33 ($m = 9$)	(see FR-2.1.5)
7	Decaphene	$(C_6)_{10}$	*cf.* 30 ($n = 10$)	(see FR-2.1.3)
8	Decacene	$(C_6)_{10}$	*cf.* 40 ($n = 10$)	(see FR-2.1.2)
9	Decaphene	$(C_6)_{10}$	*cf.* 31 ($n = 10$)	(see FR-2.1.3)
10	Ovalene	$(C_6)_{10}$		

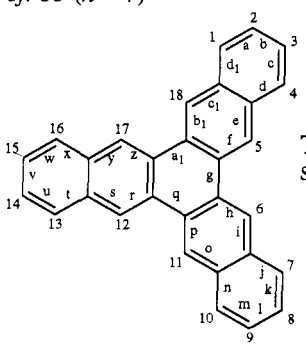


11	Decahelicene	$(C_6)_{10}$	*cf.* 32 ($n = 10$)	(see FR-2.1.7) *Note* a
12	Octaphenylene	$(C_6)_8.C_{16}$	*cf.* 33 ($m = 8$)	(see FR-2.1.5)
13	Tetranaphthylene	$(C_6)_8.C_8$	*cf.* 25 ($k = 4$)	(see FR-2.1.6)
14	Nonacene	$(C_6)_9$	*cf.* 40 ($n = 9$)	(see FR-2.1.2)
15	Nonaphene	$(C_6)_9$	*cf.* 35 ($n = 9$)	(see FR-2.1.3)
16	Nonahelicene	$(C_6)_9$	*cf.* 32 ($n = 9$)	(see FR-2.1.7) *Note* a
17	Heptaphenylene	$(C_6)_7.C_{14}$	*cf.* 33 ($m = 7$)	(see FR-2.1.5)

18	Octacene	$(C_6)_8$	*cf.* 40 (n = 8)	(see FR-2.1.2)
19	Octaphene	$(C_6)_8$	*cf.* 31 (n = 8)	(see FR-2.1.3)
20	Pyranthrene	$(C_6)_8$		

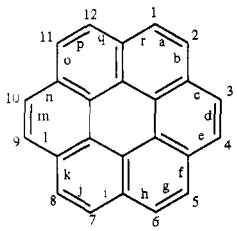


21	Octahelicene	$(C_6)_8$	*cf.* 32 (n = 8)	(see FR-2.1.7) *Note* a
22	Hexaphenylene	$(C_6)_6.C_{12}$	*cf.* 33 (m = 6)	(see FR-2.1.5)
23	Heptacene	$(C_6)_7$	*cf.* 40 (n = 7)	(see FR-2.1.2)
24	Heptaphene	$(C_6)_7$	*cf.* 35 (n = 7)	(see FR-2.1.3)
25	Trinaphthylene	$(C_6)_7$		(see FR-2.1.6)

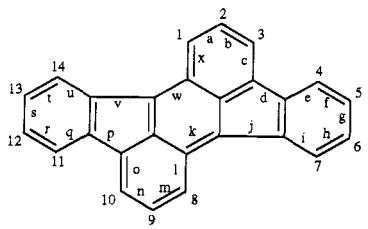


Three naphthalene systems - hence k = 3

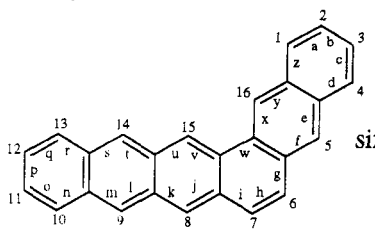
26	Coronene	$(C_6)_7$	



27	Heptahelicene	$(C_6)_7$	*cf.* 32 (n = 7)	(see FR-2.1.7) *Note* a
28	Rubicene	$(C_5)_2.(C_6)_5$		

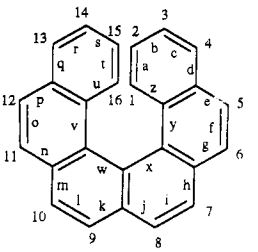


29	Pentaphenylene	$(C_6)_5.C_{10}$	*cf.* 33 (m = 5)	(see FR-2.1.5)
30	Hexacene	$(C_6)_6$	*cf.* 40 (n = 6)	(see FR-2.1.2)
31	Hexaphene	$(C_6)_6$		(see FR-2.1.3)



six rings hence n = 6

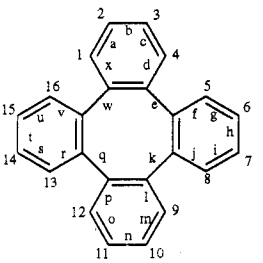
32 Hexahelicene $(C_6)_6$



(see FR-2.1.7) *Note* a

six rings hence $n = 6$

33 Tetraphenylene $(C_6)_4.C_8$

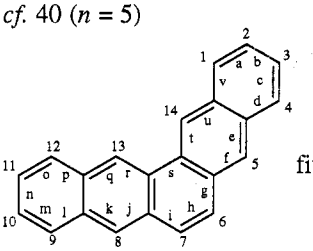


(see FR-2.1.5)

four benzene rings hence $m = 4$

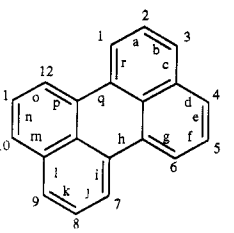
34 Pentacene $(C_6)_5$ *cf.* 40 ($n = 5$) (see FR-2.1.2)

35 Pentaphene $(C_6)_5$ (see FR-2.1.3)

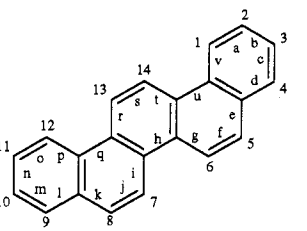


five rings hence $n = 5$

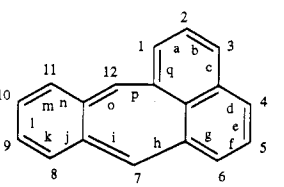
36 Perylene $(C_6)_5$



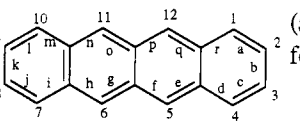
37 Picene $(C_6)_5$



38 Pleiadene $(C_6)_3.C_7$

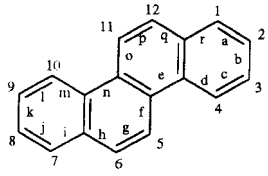
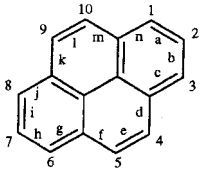
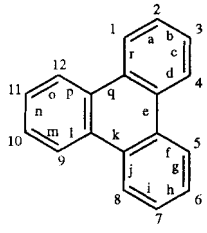
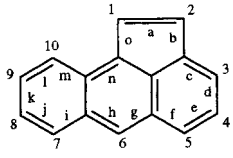
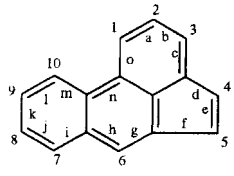
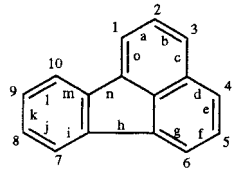
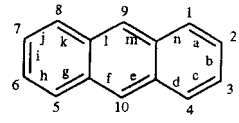
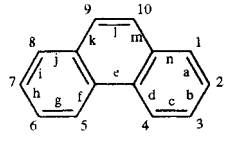
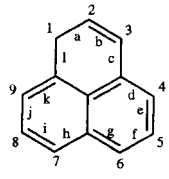


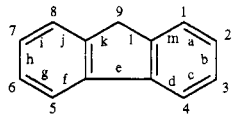
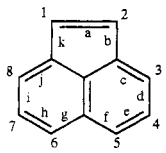
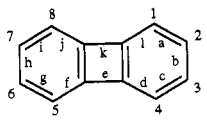
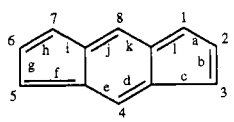
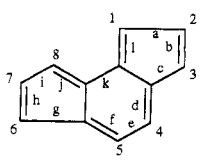
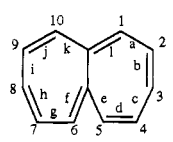
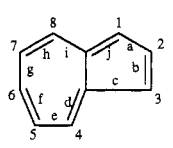
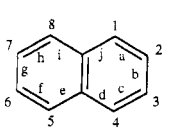
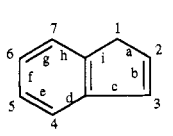
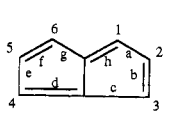
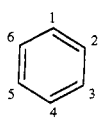
39 Tetracene $(C_6)_4$



(see FR-2.1.2) *Note* b

four rings hence $n = 4$

40	Tetraphene	$(C_6)_4$	*cf.* 26 (n = 4)	(see FR-2.1.3)
41	Chrysene	$(C_6)_4$		
42	Pyrene	$(C_6)_4$		
43	Triphenylene	$(C_6)_4$		
44	Aceanthrylene	$C_5.(C_6)_3$		
45	Acephenanthrylene	$C_5.(C_6)_3$		
46	Fluoranthene	$C_5.(C_6)_3$		
	Note c			
47	Anthracene	$(C_6)_3$		*Note* a
48	Phenanthrene	$(C_6)_3$		*Note* d
49	Phenalene (1*H*-form shown)	$(C_6)_3$		

50	Fluorene (9*H*-form shown)	$C_5.(C_6)_2$		
51	Acenaphthylene	$C_5.(C_6)_2$		
52	Biphenylene	$C_4.(C_6)_2$		*Note* e
53	*s*-Indacene	$(C_5)_2.C_6$		*Note* e
54	*as*-Indacene	$(C_5)_2.C_6$		*Note* e
55	Polyalene	$(C_n)_2$ $(n > 6)$		Heptalene ($n = 7$) shown (see FR-2.1.4)
56	Azulene	$C_5.C_7$		
57	Naphthalene	$(C_6)_2$		
58	Indene (1*H*-form shown)	$C_5.C_6$		
59	Pentalene	$(C_5)_2$		(see FR-2.1.4)
60	Polyalene	$(C_p)_2$	*cf.* 50 ($p = 3$ or 4)	(see FR-2.1.4)
61	[*p*]Annulene	C_p $(p > 6)$		*Note* f
62	Benzene	C_6		

63 [*p*]Annulene C_p ($p < 6$) *Note* g

Notes

a. Non-standard numbering.

b. Formerly called naphthacene which is still used by *CAS* and *Beilstein*..

c. *CAS* and *Beilstein* includes trindene (cyclopenta[*e*]-*as*-indacene).

d. Non-standard orientation, hence non-standard numbering.

e. In the previous edition of these rules (rule A-21.1, ref 3) indacene was preferred to biphenylene. This is now reversed to follow FR-2.3.c (see also Table 20, ref 3a).

f. These names only apply for a parent component; otherwise cycloalka is used as a fusion prefix (see FR-2.1.1).

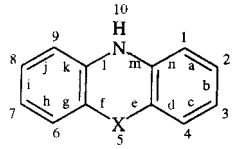
g. Only [5]annulene may be used as a parent *e.g.* cyclobuta[1,2:3,4]di[5]annulene. The prefix cycloalka- is used for attached components (see FR-2.1.1).

Appendix 2

Heterocyclic parent components in order of decreasing seniority.

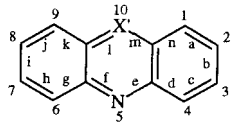
Note a

1 Phenoxazine (X = O)
2 Phenothiazine (X = S)
3 Phenoselenazine (X = Se)
4 Phenotellurazine (X = Te)

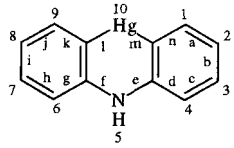


(10*H*-form shown)

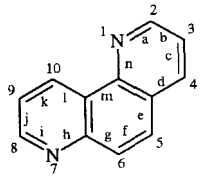
5 Phenophosphazinine (X' = P) *Note* b
6 Phenarsazinine (X' = As) *Note* c



7 Phenomercurazine (5*H* form shown) *Note* d



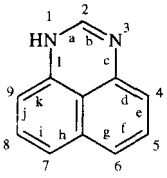
8 Phenazine (X' = N) See 5 and 6
9 1,7-Phenanthroline
10 1,8-Phenanthroline
11 1,9-Phenanthroline
12 1,10-Phenanthroline
13 2,7-Phenanthroline
14 2,8-Phenanthroline
15 2,9-Phenanthroline
16 3,7-Phenanthroline
17 3,8-Phenanthroline
18 4,7-Phenanthroline



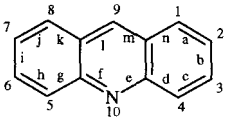
1,7-isomer shown

Note. One nitrogen atom in each of the two terminal rings, see FR-2.2.4

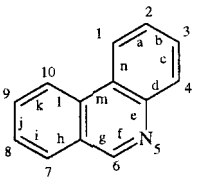
19 Perimidine (1*H*-form shown)



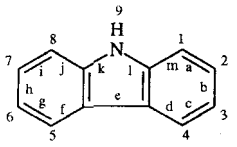
20 Acridine *Note* e



21 Phenanthridine
Note f

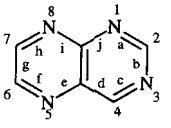


22 Carbazole
(9H-form shown)

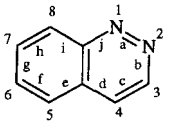


Note e

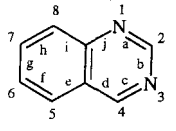
23 Pteridine



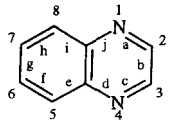
24 Cinnoline



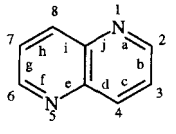
25 Quinazoline



26 Quinoxaline

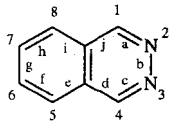


27 1,5-Naphthyridine
28 1,6-Naphthyridine
29 1,7-Naphthyridine
30 1,8-Naphthyridine



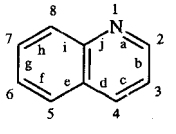
1,5-isomer shown
Note. One nitrogen atom in each ring.
see FR-2.2.4

31 Phthalazine

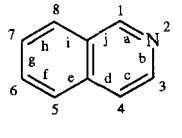


32 2,6-Naphthyridine
33 2,7-Naphthyridine
34 Quinoline

see 27-30
see 27-30
Note g

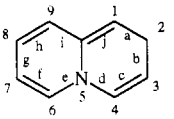


35 Isoquinoline

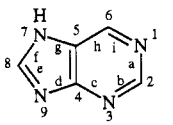


Note g

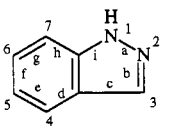
36 Quinolizine (2*H*-form shown) *Note* g



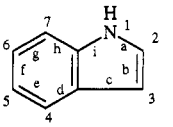
37 Purine (7*H*-form shown) *Note* e



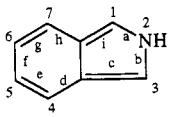
38 Indazole (1*H*-form shown)



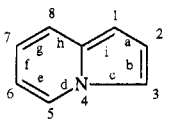
39 Indole (1*H*-form shown)



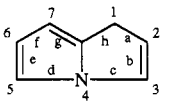
40 Isoindole (2*H*-form shown)



41 Indolizine



42 Pyrrolizine (1*H*-form shown)

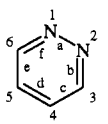


43 Seven-membered heterocyclic ring or larger with at least one nitrogen atom, *e.g.* azepine.

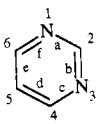
44 Six-membered heterocyclic ring with at least three heteroatoms including at least one nitrogen atom, *e.g.* 1,3,5-oxadiazine.

45 Six-membered heterocyclic ring with one nitrogen atom and a different heteroatom, *e.g.* 1,2-thiazine.

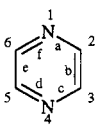
46 Pyridazine



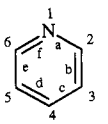
47 Pyrimidine



48 Pyrazine



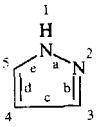
49 Pyridine



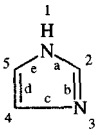
50 Five-membered heterocyclic ring with at least three heteroatoms, including at least one nitrogen atom, e.g. 1,2,5-oxadiazole (formerly called furazan).

51 Five-membered heterocyclic ring with one nitrogen atom and a different heteroatom *e.g.* 1,2-oxazole. *Note* h

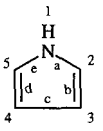
52 Pyrazole (1*H*-form shown)



53 Imidazole (1*H*-form shown)



54 Pyrrole (1*H*-form shown)



55 Three- or four-membered heterocyclic ring with at least one nitrogen atom *e.g.* azirene.

56 Heterocyclic ring with halogen but no nitrogen atom *e.g.* 1λ⁵-1,2-iodoxole

57 Phenoxathiine (X = S)

58 Phenoxaselenine (X = Se)

59 Phenoxatellurine (X = Te)

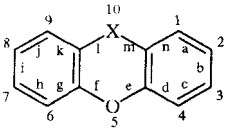
60 Phenoxaphosphinine (X = PH) *Note* i

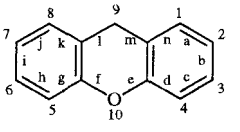
61 Phenoxarsinine (X = AsH) *Note* j

62 Phenoxastibinine (X = SbH) *Note* k

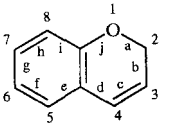
63 Oxanthrene (X = O) *Note* l

64 Xanthene (9*H*-form shown) *Note* e

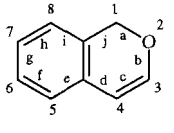




65 Chromene (2*H*-form shown) *Note* m



66 Isochromene (1*H*-form shown) *Note* n

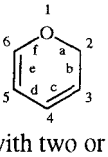


Note o

67 Seven-membered heterocyclic ring or larger with at least one oxygen atom (no nitrogen atom; see 43) *e.g.* oxepine.

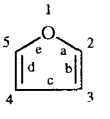
68 Six-membered heterocyclic ring with two or more heteroatoms at least one of which is oxygen (no nitrogen atom; see 44, 45) *e.g.* 1,4-dioxine

69 Pyran (2*H*-form shown)



70 Five-membered heterocyclic ring with two or more heteroatoms at least one of which is oxygen (no nitrogen atom; see 50-51) *e.g.* 1,3-dioxole.

71 Furan



72 Three or four-membered heterocyclic ring with at least one oxygen atom (no nitrogen atom; see 55) *e.g.* oxirene.
73 Phenothiarsinine see 57-63, X = AsH, S instead of O *Note* p
74 Thianthrene see 57-63, X = S, S instead of O
75 Thioxanthene see 64, S instead of O *Note* e
76 Thiochromene see 65, S instead of O *Note* m
77 Isothiochromene see 66, S instead of O *Note* n
78 Heteromonocyclic ring with at least one sulfur atom (no nitrogen or oxygen atoms). The trivial names thiophene (see 71, S instead of O) and thiopyran (see 69, S instead of O) are retained.
79 Selanthrene see 57-63, X = Se, Se instead of O
80 Selenoxanthene see 64, Se instead of O *Note* e
81 Selenochromene see 65, Se instead of O *Note* m
82 Isoselenochromene see 66, Se instead of O *Note* n
83 Heteromonocyclic ring with at least one selenium atom (no N, O or S atoms) The trivial name selenophene (see 71, Se instead of O) is retained.
84 Telluranthrene see 57-63, X = Te, Te instead of O
85 Telluroxanthene see 64, Te instead of O *Note* e
86 Tellurochromene see 65, Te instead of O *Note* m
87 Isotellurochromene see 66, Te instead of O *Note* n
88 Heteromonocyclic ring with at least one tellurium atom (no N, O, S, or Se aoms). The trivial name tellurophene (see 71, Te instead of O) is retained.
89 Phosphanthrene see 5, 6, & 8, X' = P, P instead of N
90 Acridophosphine see 5, 6, & 8, X' = CH, P instead of N *Note* q
91 Phosphanthridine see 21, P instead of N
92 Phosphinoline see 34, P instead of N
93 Isophosphinoline see 35, P instead of N
94 Phosphinolizine, see 36, P instead of N
95 Phosphindole see 39, P instead of N
96 Isophosphindole see 40, P instead of N
97 Phosphindolizine, see 41, P instead of N
98 Heteromonocyclic ring with at least one phosphorus atom (no N, O, S, Se or Te atoms).
99 Arsanthrene see 5, 6, & 8, X' = As, As instead of N
100 Acridarsine see 5, 6, & 8, X' = CH, As instead of N *Note* q
101 Arsanthridine see 21, As instead of N
102 Arsinoline see 34, As instead of N
103 Isoarsinoline see 35, As instead of N
104 Arsinolizine, see 36, As instead of N
105 Arsindole see 39, As instead of N
106 Isoarsindole see 40, As instead of N
107 Arsindolizine, see 41, As instead of N
108 Heteromonocyclic ring with As, and Sb, Bi, Si, Ge, Sn, Pb, B, Hg as possible heteroatoms.
109 Silanthrene see 5, 6, & 8, X' = SiH, SiH instead of N
110 Boranthrene see 5, 6, & 8, X' = B, B instead of N)
111 Mercuranthrene see 57-63, X = Hg, Hg instead of O *Note* r

Notes.

a. *CAS* includes ten additional fusion parent components which have higher priority. In order of preference they are:

Anthrazine	(dinaphtho[2,3-*a*:2',3'-*h*]phenazine)
Phenanthrazine	(tetrabenzo[*a,c,h,j*]phenazine)
Triphenodioxazine	(dibenzo[*e,e'*]benzo[1,2-*b*:4,5-*b'*]bis[1,4]oxazine)
Triphenodithiazine	(dibenzo[*e,e'*]benzo[1,2-*b*:4,5-*b'*]bis[1,4]thiazine)
Phthaloperine	(isoindolo[2,1-*a*]perimidine)
Acrindoline	(indolo[3,2-*e*]acridine)
Thebenidine	(benzo[*lmn*]phenanthridine)
Quinindoline	(indolo[2,3-*b*]quinoline)
Quindoline	(indolo[3,2-*b*]quinoline)
Anthyridine	(pyrido[2,3-*b*][1,8]naphthyridine)

b. Formerly called phenophosphazine

c. Formerly called phenoarsazine

d. Formerly called phenomercazine; *CAS* calls 2*H*-phenomercurazine (3,6-cyclohexadien-1-yl-2-ylidene-nitrilo-1,2-phenylene)mercury.

e. Non-standard numbering.

f. β-Carboline (pyrido[3,4-*b*]indole) was abandoned as a fusion parent component in the 4th edition of section B (ref 3).

g. *CAS* retains the traditional order quinolizine preferred to quinoline, preferred to isoquinoline.

h. Isoxazole, oxazole, isothiazole, thiazole, isoselenazole, selenazole, isotellurazole and tellurazole are now named as Hantzsch-Widman heterocycles (1,2-oxazole, 1,3-oxazole, 1,2-thiazole, 1,3-thiazole *etc.*) but were formerly used as components. They are still used by *CAS* and *Beilstein*.

i. Formerly called phenoxaphosphine as used by *CAS*.

j. Formerly called phenoxarsine as used by *CAS*.

k. Formerly called phenoxantimonine as used by *CAS*.

l. Formerly called dibenzo[*b*,*e*][1,4]dioxine. *CAS* uses dibenzo[*b*,*e*][1,4]dioxin, *Beilstein* uses dibenzo[1,4]dioxine.

m. Called 1-benzopyran by *CAS*. Similarly *CAS* uses 1-benzothiopyran, 1-benzoselenin and 1-benzotellurin for the chalcogen analogues.

n. Called 2-benzopyran by *CAS*. Similarly *CAS* uses 2-benzothiopyran, 2-benzoselenin and 2-benzotellurin for the chalcogen analogues.

o. Benzofuran and isobenzofuran are no longer used as fusion parent components. *CAS* still uses both whereas *Beilstein* uses both for the unmodified ring system but only furan for further fusion.

p. Formerly called phenothiarsine.

q. Standard numbering [not as acridine (20)] (Ref 3a is in error on this point).

r. Formerly called phenomercurin or phenomercurine; *CAS* and *Beilstein* calls mercuranthrene cyclo-di-μ-1,2-phenylenedimercury.