

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY  
ORGANIC CHEMISTRY DIVISION

Commission on Nomenclature of Organic Chemistry

PHANE NOMENCLATURE

PART II: SUBSTITUTION DERIVATIVES OF PHANE PARENT HYDRIDES

(IUPAC Recommendations 2001)

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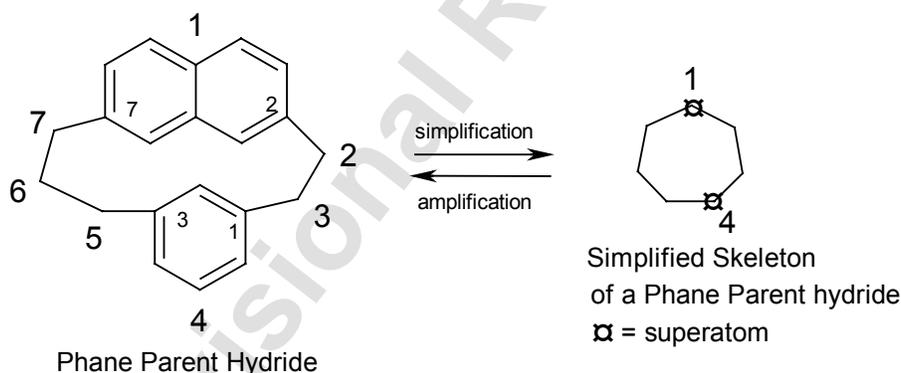
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## Synopsis

Cyclophane and linear phane systems are considered as parent hydrides. Their derivatives are named in conformity with the principles, rules and conventions prescribed for naming organic compounds. The following nomenclatural features are described: indicated and added hydrogen, order of seniority for numbering, substituents expressed as suffixes, substituents cited as prefixes, phane parent hydrides modified by addition or subtraction of hydrogen atoms, polyfunctional derivatives.

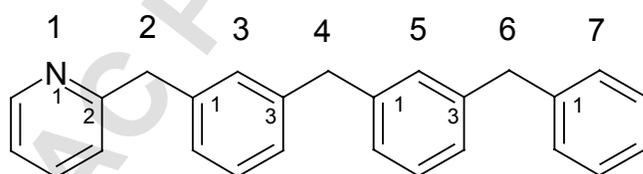
## Introduction

Phane nomenclature is a new method for building names for organic structures by assembling names that describe component parts of a complex structure (ref. 1). It is based on the idea that a relatively simple skeleton for a parent hydride structure can be modified by an operation called "amplification", a process that replaces one or more special atoms (superatoms) of the simplified skeleton by multiatomic structure(s). The multiatomic structure is a fully saturated or a "mancude" ring or ring system. In the amplification operation each superatom is replaced by an amplificant denoted by an "amplification prefix" attached to a stem called a "simplified skeletal name". The latter ends with the term "phane" and is formed according to the principles for deriving names of saturated hydrocarbons. Accordingly, all of the atoms implied by the skeletal name, except for those replaced by amplification prefixes are, by convention, saturated carbon atoms. An amplification prefix is derived from the name of the corresponding cyclic parent hydride by the addition of the terminal letter "a" with elision of a terminal vowel of the parent hydride name, if present. Phane prefixes thus resemble the prefixes, such as "oxa", "aza", etc., that indicate replacement of a single atom, usually a carbon atom, by a different atom.

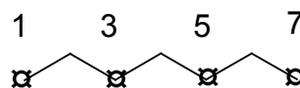


Simplified skeletal name: cycloheptaphane

Phane parent hydride name: 1(2,7)-naphthalena-4(1,3)-benzenacycloheptaphane



Phane Parent Hydride



Simplified Skeleton  
of a Phane parent hydride  
α = superatom

Simplified skeletal name: heptaphane

Phane parent hydride name: 1(2)-pyridina-3,5(1,3),7(1)-tribenzenaheptaphane

The locants in front of the parentheses in the phane parent hydride name identify the positions of the superatoms in the simplified skeleton that are replaced by the ring structure specified by the amplification prefix immediately following. By the same token, they also identify the positions of the rings and ring systems in the phane parent hydride. These locants are determined by the inherent numbering of the simplified skeleton and the seniority of the rings and ring systems in the phane parent hydride. The locants within the parentheses specify the atoms of the ring structure specified by the amplification prefixes that are linked to the adjacent normal atoms of the simplified parent skeleton.

In addition to the basic principles, rules and conventions of Phane Nomenclature, Part I contains the fundamental methodology for numbering phane parent hydrides and the application of skeletal replacement ('a') nomenclature for naming heterophane parent hydrides.

Part II of Phane Nomenclature describes derivatives of phane systems formed by substitutive nomenclature (ref. 2a). As parent hydrides, phane systems are totally integrated in substitutive nomenclature and therefore follow the general rules of this type of nomenclature. When required, other types of nomenclature are used to name derivatives, for example, functional class nomenclature for naming esters (ref. 2b), anhydrides (ref. 2c) and acid halides (ref. 2d).

## Contents

- PhII-1. Numbering
- PhII-2. Specification of indicated hydrogen
- PhII-3. Substituent groups derived from phane parent hydrides
- PhII-4. Substitutive nomenclature forphanes
- PhII-5. Phane parent hydrides modified by the addition or subtraction of hydrogen atoms
- PhII-6. Polysubstituted derivatives of phane parent hydrides

## PhII-1 Numbering

**PhII-1.1** Insofar as the general rules of substitutive nomenclature leave a choice, the starting point and direction of numbering of a compound are chosen so as to give lowest locants to the following structural features (if present) considered successively in the order listed until a decision is reached (ref. 2e).

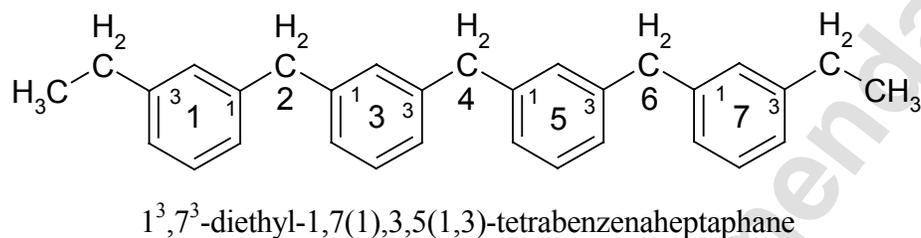
- (a) numbering of phane parent hydrides
- (b) heteroatoms introduced by skeletal 'a' replacement
- (c) indicated hydrogen
- (d) nondetachable hydro-dehydro prefixes
- (e) principal characteristic group named as suffix
- (f) unsaturation (ene/yne endings)
- (g) substituents named as prefixes (alphabetized substituents)

**PhII-1.2** In these recommendations, 'hydro-' and 'dehydro-' prefixes are classified as non-detachable (ref. 2f). Since nondetachable hydro prefixes define specific parent hydrides, they take precedence for low locants over substituent groups, but not over indicated hydrogen. Hydro and dehydro prefixes are cited in names immediately in front of the name of the phane parent hydride, or in front of 'a' replacement prefixes, when present.

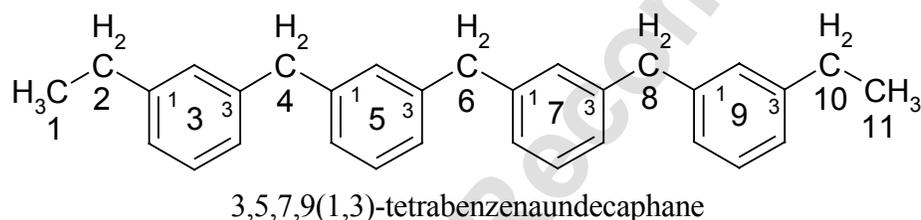
**PhII-1.3** Also, when there is a choice, the established procedure for lowest locants is applied. The lowest locant set (ref. 2g) is the one that has the lowest numerical value at the first point of difference when the sets are compared term by term in order of increasing numerical value.

**PhII-1.4** Acyclic phane parent hydrides are, by definition, terminated by an amplificant at each end of the acyclic phane system. Alkyl substituents on these terminal amplificants do not extend the phane system beyond the terminal amplificants. Names are constructed in conformity with Section PhI-3.3 (ref. 1b).

Examples:



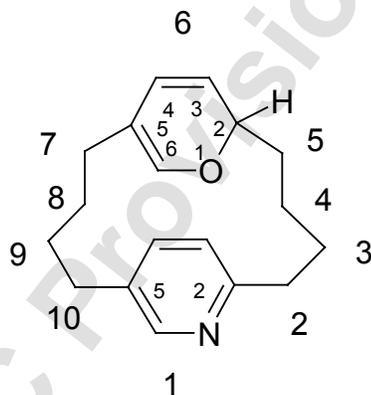
NOT



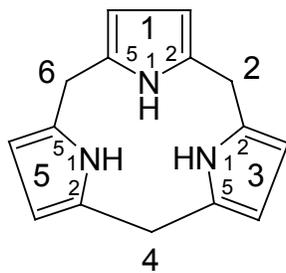
## PhII-2 Specification of indicated hydrogen

Indicated hydrogen, when present in an amplificant, is placed before the phane parent hydride name and preceded by appropriate locants (ref. 2h).

Examples:



$6^2H$ -1(2,5)-pyridina-6(2,5)-pyranacyclodecaphane



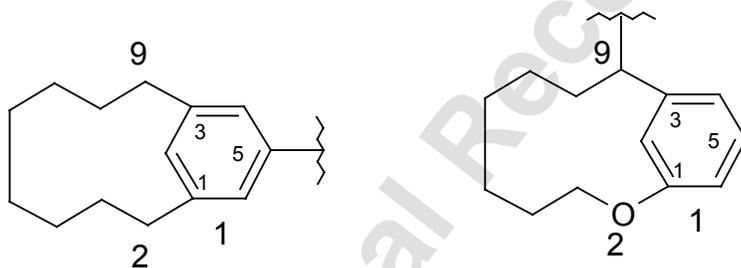
1<sup>1</sup>H,3<sup>1</sup>H,5<sup>1</sup>H-1,3,5(2,5)tripyrolacyclohexaphane

### PhII-3 Substituent groups derived from phane parent hydrides

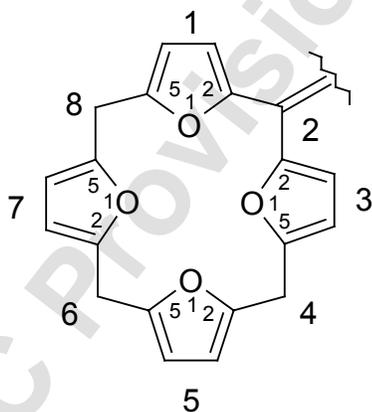
#### PhII-3.2 General method

Names of substituent groups derived from phane parent hydrides are formed in accordance with the general methods (ref. 2i). The suffixes '-yl', and '-ylidene' are added to the name of the phane parent hydride preceded by appropriate locants. Low locants are assigned to these suffixes in accordance with the fixed numbering of the phane parent hydride or phane parent hydrides modified by skeletal replacement ('a') nomenclature. If a choice is possible, low locants are assigned to the suffix '-yl'. In names, the suffix '-yl' precedes '-ylidene'.

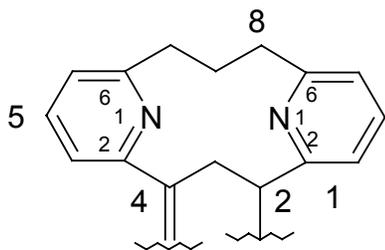
Examples:



1(1,3)-benzenacyclononaphan-1<sup>5</sup>-yl    2-oxa-1(1,3)-benzenacyclononaphan-9-yl



1,3,5,7(2,5)-tetrafuracyclooctaphan-2-ylidene

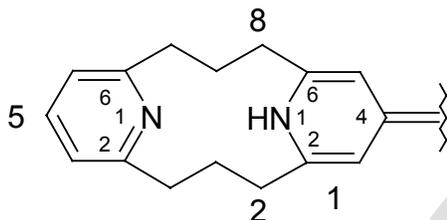


1,5(2,6)-dipyridinacyclooctaphan-2-yl-4-ylidene

**PhII-3.2** The ‘added hydrogen method’

The added hydrogen method is applied when ‘-ylidene’ free valences are attached to a mancude ring or ring system (ref. 2i). The method called the ‘added hydrogen method’ describes hydrogen atoms added to a specific structure as a consequence of the addition of a suffix describing a structural modification. This type of indicated hydrogen is normally cited in parentheses after the locant of the additional structural feature. This type of compound may also be named by using nondetachable hydro prefixes.

Example



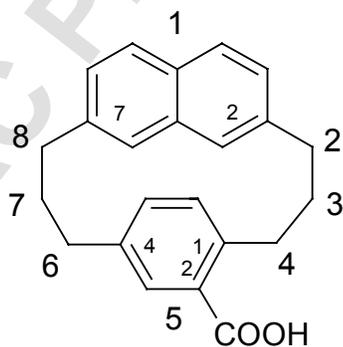
1,5(2,6)-dipyridinacyclooctaphan-1<sup>4</sup>(1<sup>1H</sup>)-ylidene (‘added hydrogen method’)  
 1<sup>1</sup>,1<sup>4</sup>-dihydro-1,5(2,6)-dipyridinacyclooctaphan-1<sup>4</sup>-ylidene (nondetachable hydro prefix method)

**PhII-4 Substitutive nomenclature forphanes**

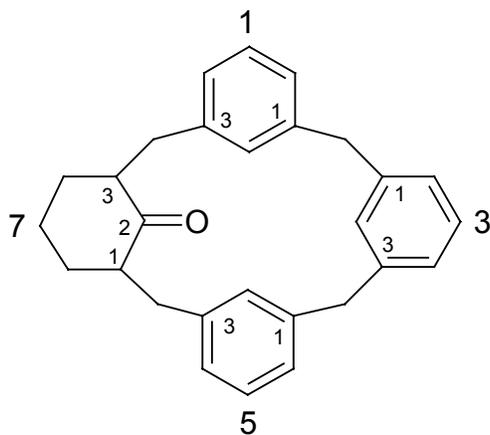
**PhII-4.1** Phanes with characteristic group suffixes

In accordance with the fixed numbering of a phane parent hydride or phane parent hydrides modified by skeletal replacement (‘a’) nomenclature, characteristic groups cited as suffixes receive lowest possible locants (see PhII-1.1).

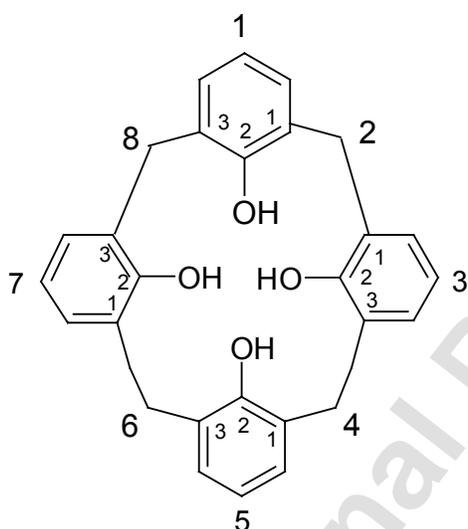
Examples:



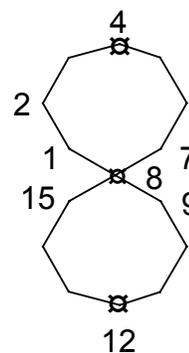
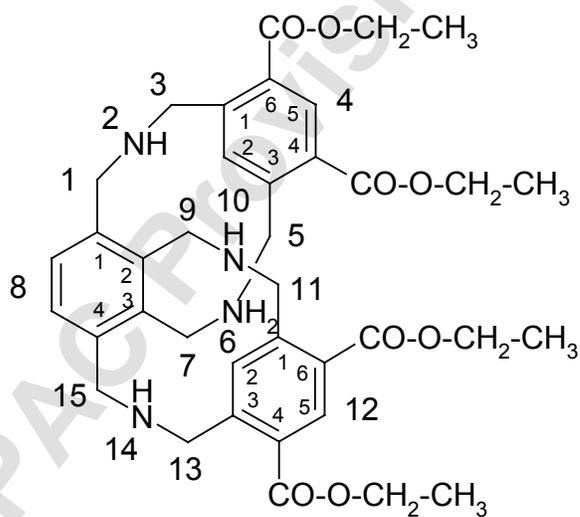
1(2,7)-naphthalena-5(1,4)-benzenacyclooctaphane-5<sup>2</sup>-carboxylic acid



1,3,5(1,3)tribenzena-7(1,3)-cyclohexanacyclooctaphan-7<sup>2</sup>-one

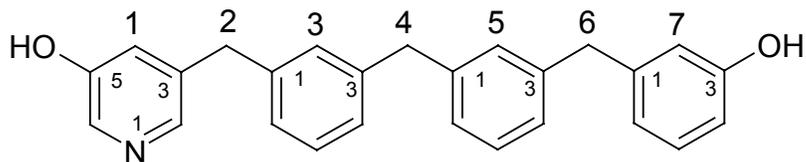


1,3,5,7(1,3)-tetrabenzenacyclooctaphane-1<sup>2</sup>,3<sup>2</sup>,5<sup>2</sup>,7<sup>2</sup>-tetrol

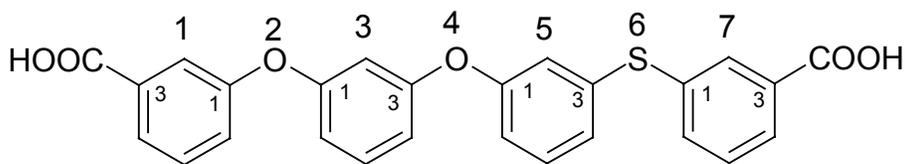


simplified skeleton  
 ☒ = superatom

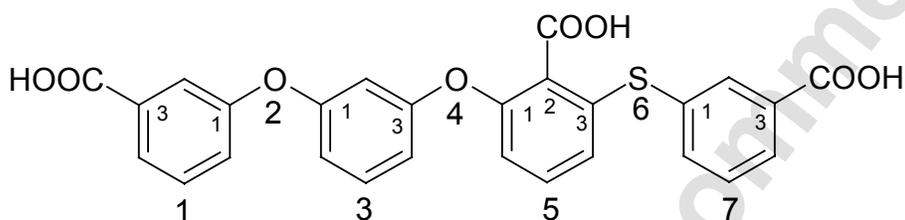
tetraethyl 2,6,10,14-tetraaza-4,12(1,3),8(1,3,2,4)-tribenzenaspiro[7.7]pentadecaphane-4<sup>4</sup>,4<sup>6</sup>,12<sup>4</sup>,12<sup>6</sup>-tetracarboxylate



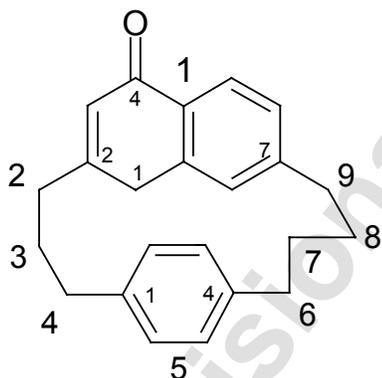
1(3)-pyridina-3,5(1,3),7(1)-tribenzenaheptaphane-1<sup>5</sup>,7<sup>3</sup>-diol



2,4-dioxa-6-thia-1,7(1),3,5(1,3)-tetrabenzenaheptaphane-1<sup>3</sup>,7<sup>3</sup>-dicarboxylic acid



2,4-dioxa-6-thia-1,7(1),3,5(1,3)-tetrabenzenaheptaphane-1<sup>3</sup>,5<sup>2</sup>,7<sup>3</sup>-tricarboxylic acid

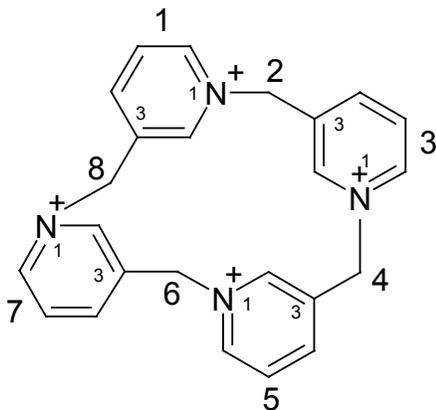


1(2,7)-naphthalena-5(1,4)-benzenacyclononaphane-1<sup>4</sup>(1<sup>1</sup>H)-one (added hydrogen method)  
 1<sup>1</sup>,1<sup>4</sup>-dihydro-1(2,7)-naphthalena-5(1,4)-benzenacyclonaphan-1<sup>4</sup>-one (nondetachable  
 hydro prefix method; see PhII-3.2)

#### PhII-4.2 Radicals and ions derived from phane parent hydrides

Radicals are named by the same method that is used for naming substituent groups, described in PhII-3. Ions may be named by use of ionic suffixes (ref. 3a).

Example:



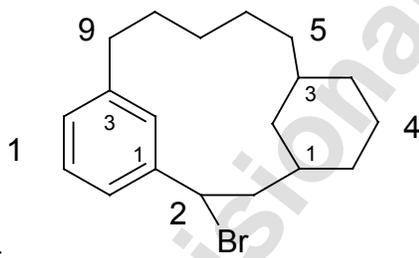
1<sup>1</sup>λ<sup>5</sup>,3<sup>1</sup>λ<sup>5</sup>,5<sup>1</sup>λ<sup>5</sup>,7<sup>1</sup>λ<sup>5</sup>-1(1,3),3,5,7(3,1)-tetrapiyridinacyclooctaphane-1<sup>1</sup>,3<sup>1</sup>,5<sup>1</sup>,7<sup>1</sup>-  
tetrakis(ylium) (preferred)  
1<sup>1</sup>,3<sup>1</sup>,5<sup>1</sup>,7<sup>1</sup>-tetraazonia-1,3,5,7(1,3)-tetrabenzenacyclooctaphane

*Note:* See ref.3a for preference of the suffix ‘-ylium’ over skeletal replacement (‘a’) prefixes.

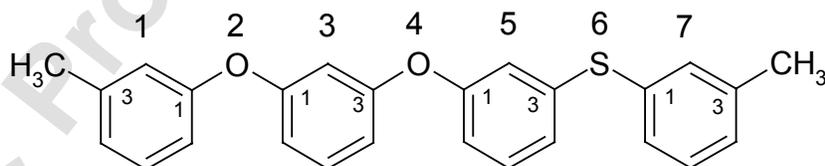
#### PhII-4.3 Substituents cited as prefixes

**PhII-4.3.1** Atoms and/or groups cited as detachable alphabetized prefixes are assigned positions according to the fixed numbering of phane parent hydride or phane parent hydrides modified by skeletal replacement (‘a’) nomenclature (ref. 2j).

Examples



2-bromo-1(1,3)-benzena-4(1,3)cyclohexanacyclononaphane

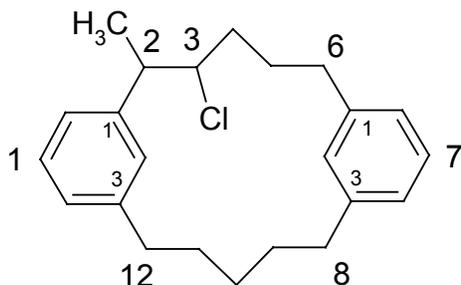


1<sup>3</sup>,7<sup>3</sup>-dimethyl-2,4-dioxa-6-thia-1,7(1),3,5(1,3)-tetrabenzenaheptaphane

When a choice is necessary, the following criteria are considered in order until a decision is made.

**PhII-4.3.2** Low locants are assigned to the prefixes considered together as a set in ascending numerical order.

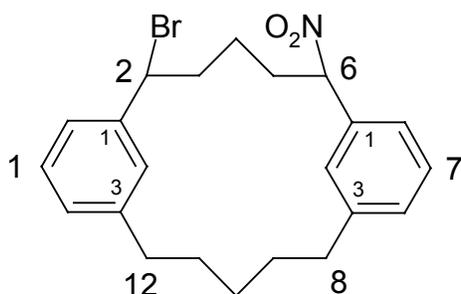
Example:



3-chloro-2-methyl-1,7(1,3)-dibenzenacyclododecaphane

**PhII-4.3.3** Low locants are allocated in the order of citation.

Example:



2-bromo-6-nitro-1,7(1,3)-dibenzenacyclododecaphane

**PhII-5 Phane parent hydrides modified by the addition or subtraction of hydrogen atoms**

Phane parent hydrides are composed of mancude (maximum number of noncumulated double bonds) and saturated cyclic components, i.e., amplificants, and alternating chains. The degree of hydrogenation of each component can be modified by applying the general rules recommended in the 1993 *Guide to IUPAC Nomenclature of Organic Compounds* by using the prefix 'hydro-' (ref 2k) to indicate the addition of hydrogen atoms; the prefix 'dehydro-' to indicate the removal of hydrogen atoms (ref 2m); and the endings '-ene' and '-yne' (2n) to denote the subtraction of hydrogen atoms. The rule of lowest locants is always applied, as indicated below for specific cases.

The following rules are applied, in the order given, until a decision is reached.

**PhII-5.1** Hydro prefixes

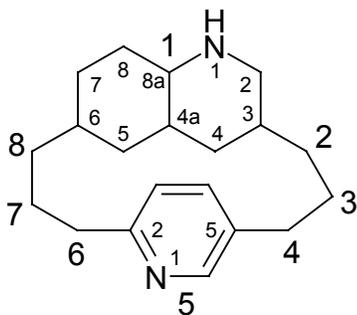
When the name of an amplificant implies the presence of the maximum number of noncumulative double bonds, other higher states of hydrogenation are indicated by use of the prefix 'hydro-', signifying the addition of one hydrogen atom, together with an appropriate numerical prefix indicating the number of hydrogen atoms added (ref. 2k). Indicated hydrogen, if required by the parent hydride, is cited in front of the name of the phane parent hydride (see PhII-2). This method is applied as follows:

Hydro prefixes are used to modify mancude monocyclic heterocycles having retained names or named in accordance with the extended Hantzsch-Widman method (for monocyclic rings having three to ten members, see ref. 2k). However, names for the fully saturated corresponding monocycles that are retained names or Hantzsch-Widman names are preferred to those expressed by hydro prefixes, for example, oxolane is preferred to tetrahydrofuran and piperidine to hexahydropyridine (ref. 1a);

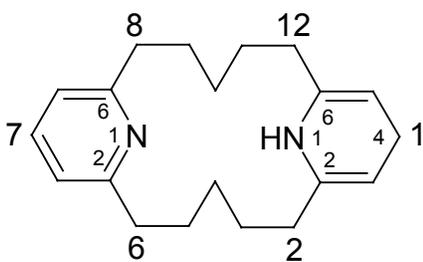
Hydro prefixes are used to indicate all modifications of the degree of unsaturation of polycyclic carbocyclic or heterocyclic mancude parent hydrides. Retained names of partially hydrogenated

parent hydrides, such as indane, chromane, isochromane, indoline and isoindoline, are not recommended as modified amplificants in phane systems (ref. 1a).

Examples:



1<sup>1</sup>,1<sup>2</sup>,1<sup>3</sup>,1<sup>4</sup>,1<sup>4a</sup>,1<sup>5</sup>,1<sup>6</sup>,1<sup>7</sup>,1<sup>8</sup>,1<sup>8a</sup>-decahydro-1(3,6)quinolina-5(5,2)-pyridinacyclooctaphane

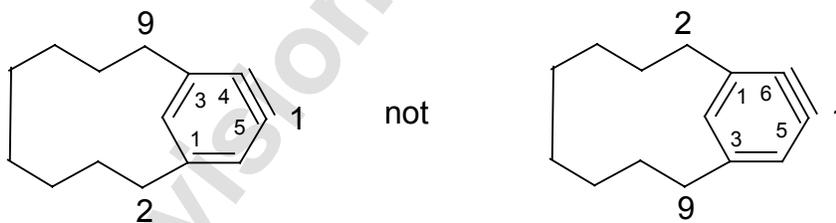


1<sup>1</sup>,1<sup>4</sup>-dihydro-1,7(2,6)-dipyridinacyclododecaphane

### PhII-5.2 Dehydro prefixes

Dehydro prefixes are used to indicate the removal of two contiguous hydrogen atoms from a mancude amplificant of a phane parent hydride system (ref. 2m).

Example:



1<sup>4</sup>,1<sup>5</sup>-didehydro-1(1,3)-benzenacyclononaphane      1<sup>5</sup>,1<sup>6</sup>-didehydro-1(1,3)-benzenacyclononaphane

### PhII-5.3 Ene and yne endings

**PhII-5.3.1** The presence of one or more double or triple bonds in an otherwise saturated phane parent hydride (except in amplificants with Hantzsch-Widman names) is denoted by changing the final 'e' of the phane parent hydride name to '-ene' or '-yne', with appropriate multiplying prefixes to indicate the multiplicity of each type of unsaturated sites (ref. 2n).

The general method must, however, be adapted to phane nomenclature names, in which the term 'phane' is considered invariant to preserve the specificity of the class. As a consequence, the endings '-ene' and '-yne' are added to a phane name, with the appropriate multiplying prefixes, with elision of the letter 'e' in the 'phane' ending before the vowels 'e' and 'y'.

In phane nomenclature, the endings ‘-ene’ and ‘-yne’ are used to denote the presence of double and triple bonds in amplificants (saturated rings and ring systems) and in the simplified skeletons.

### PhII-5.3.2 Double bonds in amplificants and in simplified phane skeletons

Low locants are allocated for double bonds in accordance with the fixed numbering of phane parent hydrides and phane parent hydrides that are modified by skeletal replacement (‘a’) nomenclature. Traditionally, the degree of unsaturation in a benzene ring is never modified by using hydro prefixes; rather, cyclohexane is used as the amplificant name and later modified by changing the ending ‘-ane’ to ‘-ene’, ‘diene’, and ‘-yne’, as required.

Three kinds of locants are required to fully describe the compounds derived from phane parent hydrides:

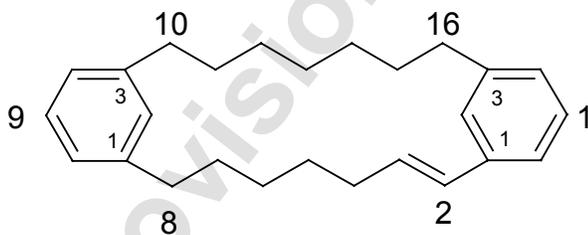
- (1) primary locants, i.e., those that denote the atoms and superatoms of the phane parent skeleton; in the structures herein they are the locants expressed by large arabic numbers (ref. 1b);
- (2) composite locants, i.e., primary locants with a superscript locant, denoting the positions in amplificants; in the structures herein they are expressed by small arabic numbers (ref. 1b);
- (3) compound locants are primary or composite locants followed by another locant enclosed in parentheses indicating that a double bond is not located between two contiguous locants (ref. 2n).

In Phane Nomenclature, double bonds are denoted in two ways:

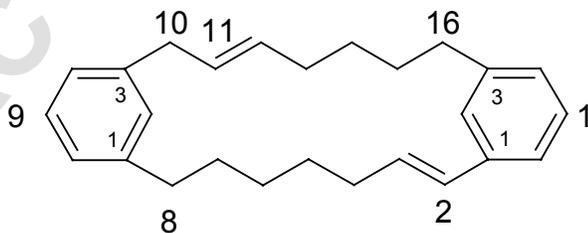
- (1) by the lowest locant assigned to a double bond when the two contiguous locants are primary locants.
- (2) by a compound locant, when one or the two locants are composite locants.

Low locants are assigned in the order, until a decision is reached, first to primary locants, then to composite locants in compound locants, without considering the composite locants in parentheses, and finally, to complete compound locants.

Examples:



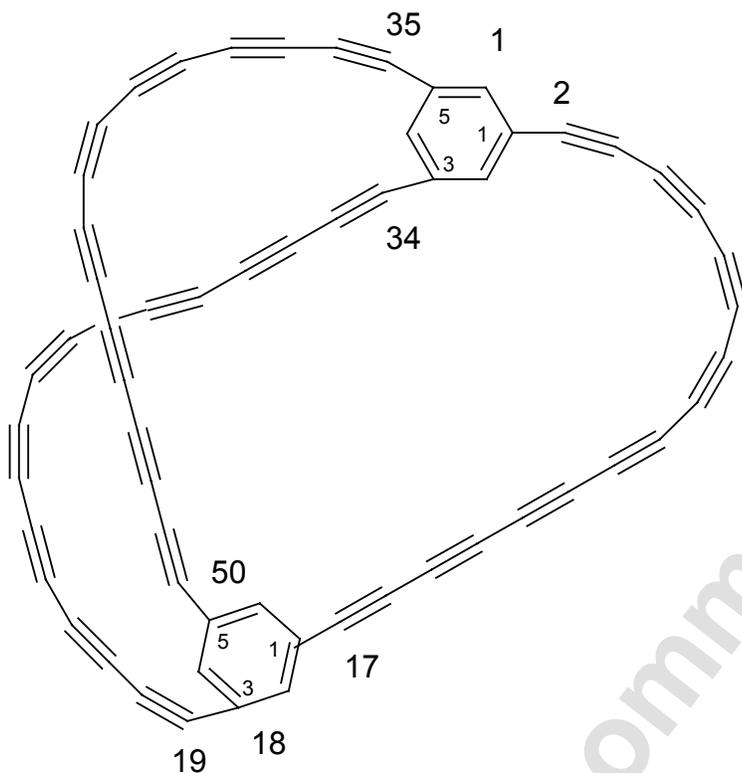
1,9(1,3)-dibenzenacyclohexadecaphan-2-ene  
(the numeral ‘2’ is a primary locant)



1,9(1,3)-dibenzenacyclohexadecaphane-2,11-diene  
(the numerals ‘2’ and ‘11’ are primary locants)



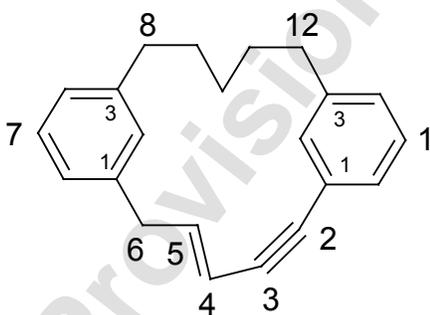




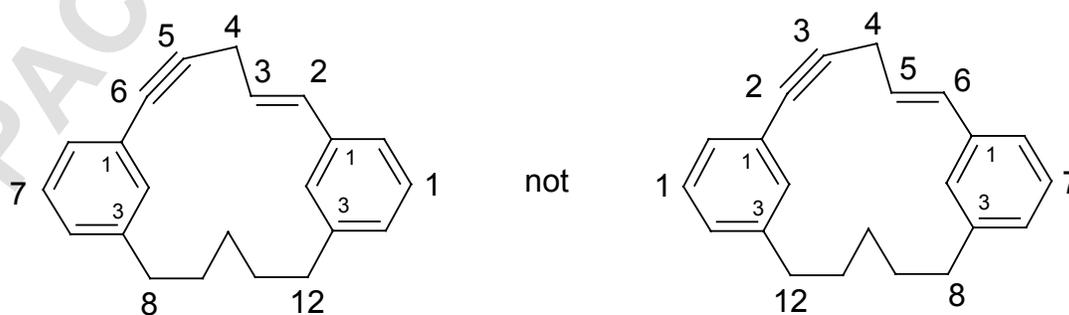
1,18(1,3,5)-dibenzenabicyclo[16.16.16]pentacontaphane-2,4,6,8,10,12,14,16,19,21,-  
23,25,27,29,31,33,35,37,39,41,43,45,47,49-tetracosayne

**PhII-5.3.4** When double and triple bonds are present in a phane system, low locants are allocated to double and triple bonds considered together; if a choice still is needed, low locants are allocated to double bonds (ref. 2n).

Examples:



1,7(1,3)-dibenzenacyclododecaphan-4-en-2-yne

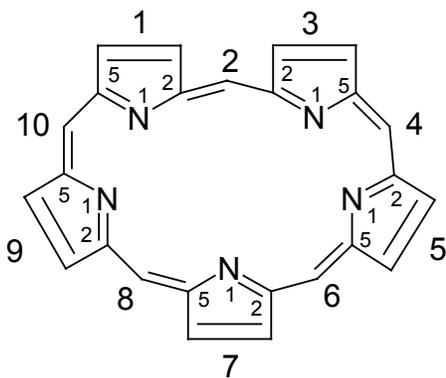


1,7(1,3)-dibenzenacyclododecaphan-2-en-5-yne 1,7(1,3)-dibenzenacyclododecaphan-5-en-2-yne

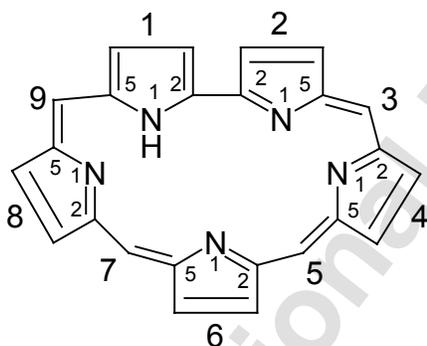
#### PhII-5.4 Double bonds between manucude amplificants and alternating atoms or chains

Double bonds between manucude amplificants having indicated hydrogen atoms and alternating atoms or chains are denoted by '-ene' endings. Any remaining indicated hydrogen atoms of the mancude amplificant are cited in front of the name and take precedence for low locants over the '-ene' endings. For the indicated hydrogen method, see ref. 4).

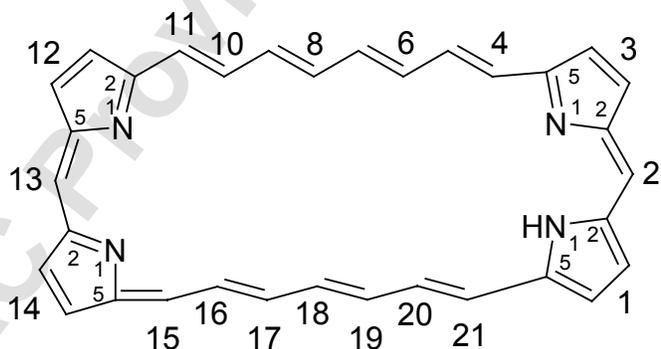
Examples:



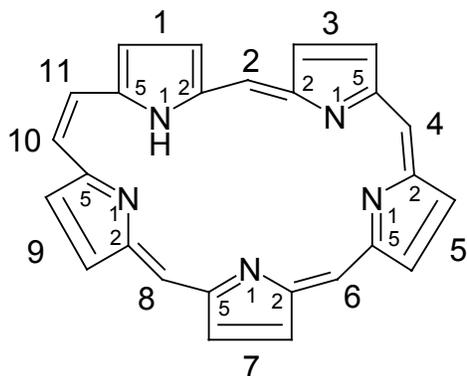
1,3,5,7,9(2,5)-pentapyrrolacyclodecaphane-1<sup>2</sup>(2),3<sup>5</sup>(4),5<sup>5</sup>(6),7<sup>5</sup>(8),9<sup>5</sup>(10)-pentaene



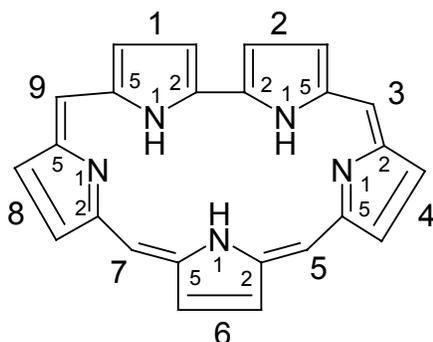
1<sup>1H</sup>-1,2,4,6,8(2,5)-pentapyrrolacyclononaphane-2<sup>5</sup>(3),4<sup>5</sup>(5),6<sup>5</sup>(7),8<sup>5</sup>(9)-tetraene



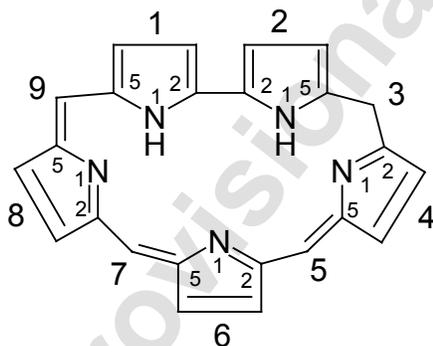
1<sup>1H</sup>-1,3,12,14(2,5)-tetrapyrrolacyclohencosaphane-2(3<sup>2</sup>),4,6,8,10,12<sup>5</sup>(13),14<sup>5</sup>(15),16,18,20-decaene



$1^1H$ -1,3,5,7,9(2,5)-pentapyrrolacycloundecaphane-2(3<sup>2</sup>),4(5<sup>2</sup>),6(7<sup>2</sup>),8(9<sup>2</sup>),10-pentaene



$1^1H,2^1H,6^1H$ -1,2,4,6,8(2,5)-pentapyrrolacyclononaphane-3(4<sup>2</sup>),5(6<sup>2</sup>),6<sup>5</sup>(7),8<sup>5</sup>(9)-tetraene  
[not  $1^1H,2^1H,6^1H$ -1,2,4,6,8(2,5)-pentapyrrolacyclononaphane-3(4<sup>2</sup>),5(6<sup>2</sup>),8<sup>5</sup>(9)-triene;  
three indicated hydrogens and four double bonds must be accounted for in the name]



$1^1H,2^1H$ -1,2,4,6,8(2,5)-pentapyrrolacyclononaphane-4<sup>5</sup>(5),6<sup>5</sup>(7),8<sup>5</sup>(9)-triene  
[not  $1^1H,2^1H,3H$ -1,2,4,6,8(2,5)-pentapyrrolacyclononaphane-4<sup>5</sup>(5),6<sup>5</sup>(7),8<sup>5</sup>(9)-  
triene; position 3 is naturally saturated in a phane structure and indicated  
hydrogen, i.e. 3H, is thus not allowed]

**PhII-5.5** Double bonds between hydrogenated mancude amplificants and alternating atoms and chains

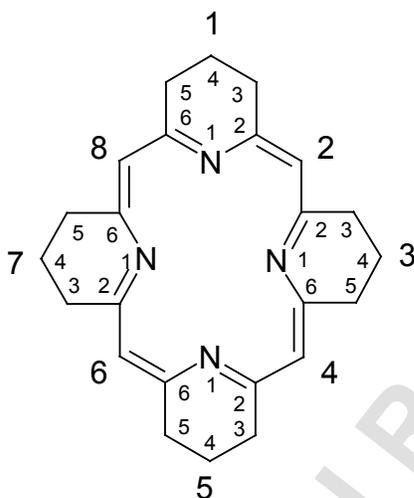
When double bonds are located between between partially or totally hydrogenated mancude amplificants and alternating atoms or chains, double bonds are denoted by the ending '-ene' and the hydrogenation of the mancude amplificant by the usual prefix 'hydro-'. Names can be formed by two methods. Method (a) is preferred

Method (a), including ‘indicated hydrogen’ atom(s). The order of operations is as follows:

- (1) Insertion of the double bonds indicated by ‘-ene’ endings and then the maximum number of double bonds in the amplificant rings;
- (2) citation of indicated hydrogen atoms, in accordance with the numbering of the amplificant;
- (3) saturation of the appropriate double bonds using ‘hydro-’ prefixes. This method for the introduction of double bonds is analogous to the method described in FR-8.1.2 (ref. 4) for introducing double bonds in bridged fused systems.

Method (b), using nondetachable ‘hydro-’ prefixes. Lowest possible locants are assigned first to indicated hydrogen, if present, then to ‘hydro-’ prefixes, and finally to double bonds denoted by the ‘-ene’ ending. (see the last example in PhII-4.1).

Example:



Method (a):  $1^4, 1^5, 3^4, 3^5, 5^4, 5^5, 7^4, 7^5$ -octahydro- $1^3H, 3^3H, 5^3H, 7^3H$ -1,3,5,7(2,6)-tetrapyrroline-cyclooctaphane- $1^2(2), 3^6(4), 5^6(6), 7^6(8)$ -tetraene

Method (b):  $1^2, 1^3, 1^4, 1^5, 3^3, 3^4, 3^5, 3^6, 5^3, 5^4, 5^5, 5^6, 7^3, 7^4, 7^5, 7^6$ -hexadecahydro-1,3,5,7(2,6)-tetrapyrroline-cyclooctaphane- $1^2(2), 3^6(4), 5^6(6), 7^6(8)$ -tetraene

Guide to name construction for these names (see structures **A**, **B**, **C**, **D**, below):

Method (a) **A** → **B** → **D**

**A** 1,3,5,7(2,6)-tetrapyrroline-cyclooctaphane

**B**  $1^3H, 3^3H, 5^3H, 7^3H$ -1,3,5,7(2,6)-tetrapyrroline-cyclooctaphane- $1^2(2), 3^6(4), 5^6(6), 7^6(8)$ -tetraene

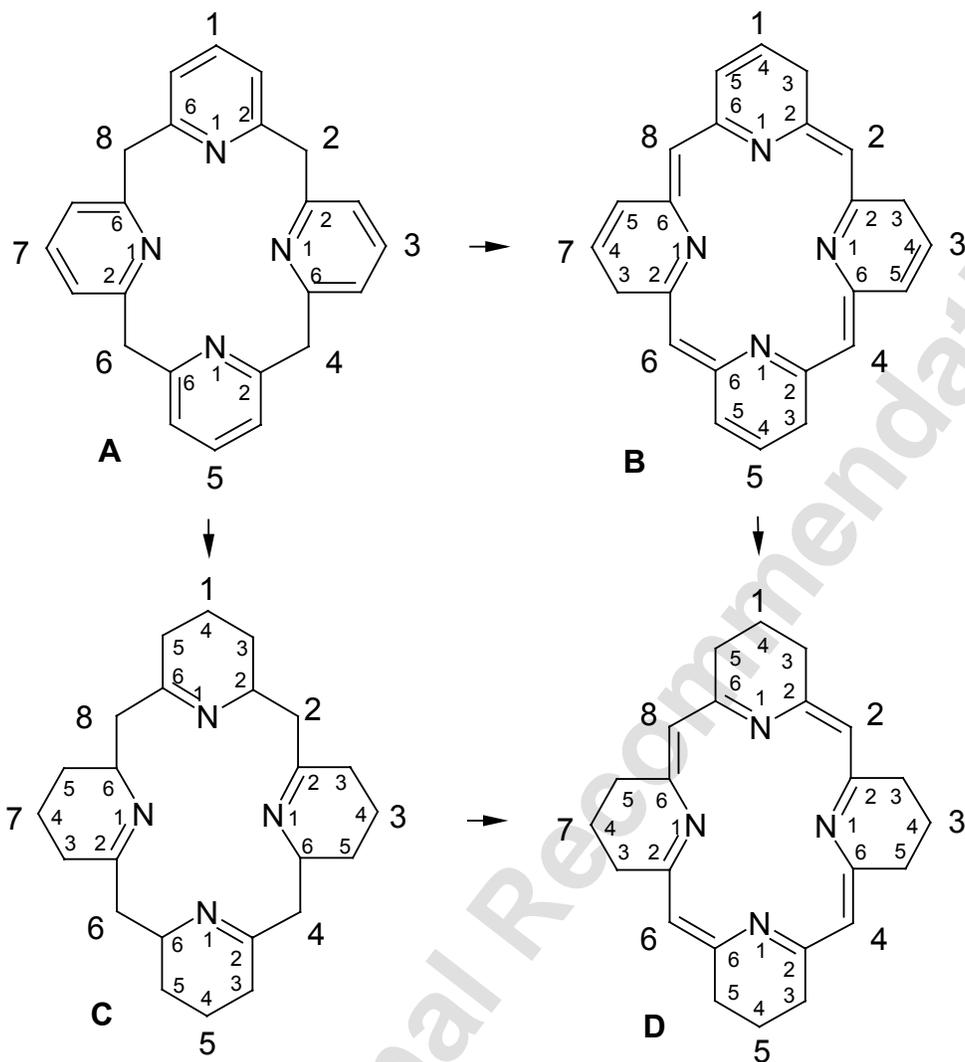
**D**  $1^4, 1^5, 3^4, 3^5, 5^4, 5^5, 7^4, 7^5$ -octahydro- $1^3H, 3^3H, 5^3H, 7^3H$ -1,3,5,7(2,6)-tetrapyrroline-cyclooctaphane- $1^2(2), 3^6(4), 5^6(6), 7^6(8)$ -tetraene

Method (b) **A** → **C** → **D**

**A** 1,3,5,7(2,6)-tetrapyrroline-cyclooctaphane

**C**  $1^2, 1^3, 1^4, 1^5, 3^3, 3^4, 3^5, 3^6, 5^3, 5^4, 5^5, 5^6, 7^3, 7^4, 7^5, 7^6$ -hexadecahydro-1,3,5,7(2,6)-tetrapyrroline-cyclooctaphane

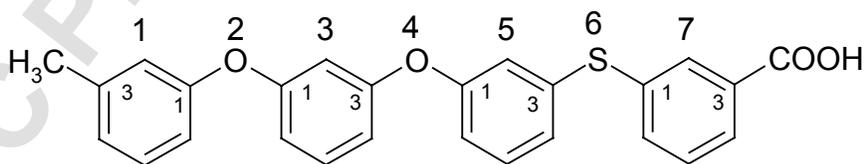
**D**  $1^2, 1^3, 1^4, 1^5, 3^3, 3^4, 3^5, 3^6, 5^3, 5^4, 5^5, 5^6, 7^3, 7^4, 7^5, 7^6$ -hexadecahydro-1,3,5,7(2,6)-tetrapyrroline-cyclooctaphane- $1^2(2), 3^6(4), 5^6(6), 7^6(8)$ -tetraene



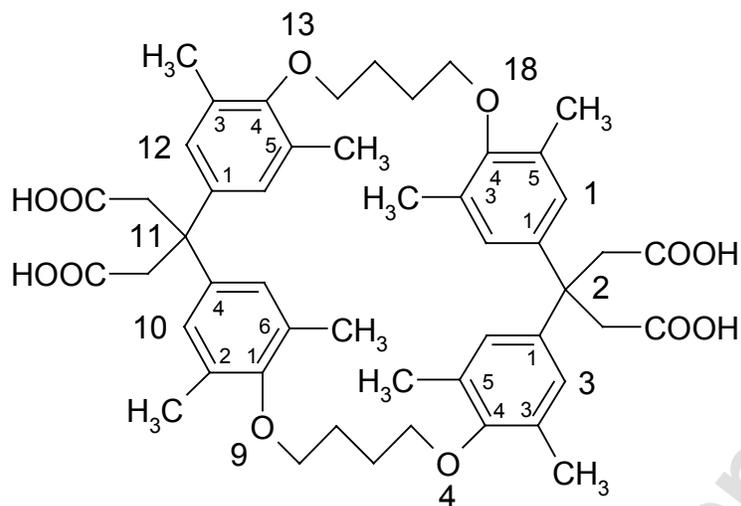
## PhII-6 Polysubstituted derivatives of phane parent hydrides

**PhII-6.1** Numbering of phane parent hydrides is based primarily on the location and nature of their amplificants and on the nature of the simplified skeleton (monocyclic, spiro, bi- and polycyclic). Locants are assigned to substituent groups in conformity with this fixed numbering. The order of priority of classes is applied to select the principal characteristic group and free valences to be cited as suffix (see Table 10, ref. 2o).

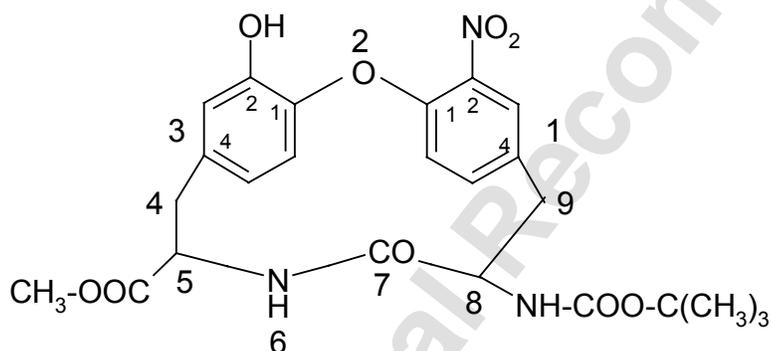
Examples:



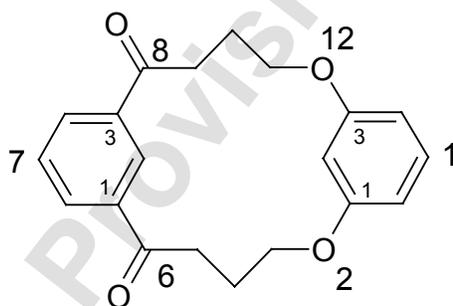
1<sup>3</sup>-methyl-2,4-dioxa-6-thia-1,7(1),3,5(1,3)-tetrabenzenaheptaphane-7<sup>3</sup>-carboxylic acid



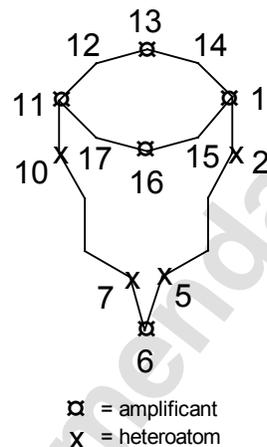
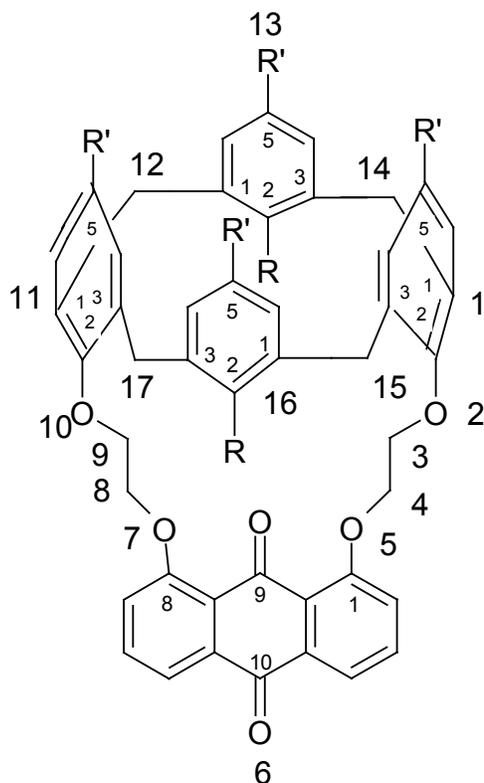
2,2',2'',2'''-(1<sup>3</sup>,1<sup>5</sup>,3<sup>3</sup>,3<sup>5</sup>,10<sup>2</sup>,10<sup>6</sup>,12<sup>3</sup>,12<sup>5</sup>-octamethyl-4,9,13,18-tetraoxa-1,3,10,12(1,4)-tetrabenzenacyclooctadecaphane-2,2,11,11-tetrayl)tetraacetic acid



methyl 8-[(*tert*-butoxycarbonyl)amino]-3<sup>2</sup>-hydroxy-1<sup>2</sup>-nitro-7-oxo-2-oxa-6-aza-1,3(1,4)-dibenzenacyclononaphane-5-carboxylate



2,12-dioxa-1,7(1,3)dibenzenacyclododecaphane-6,8-dione

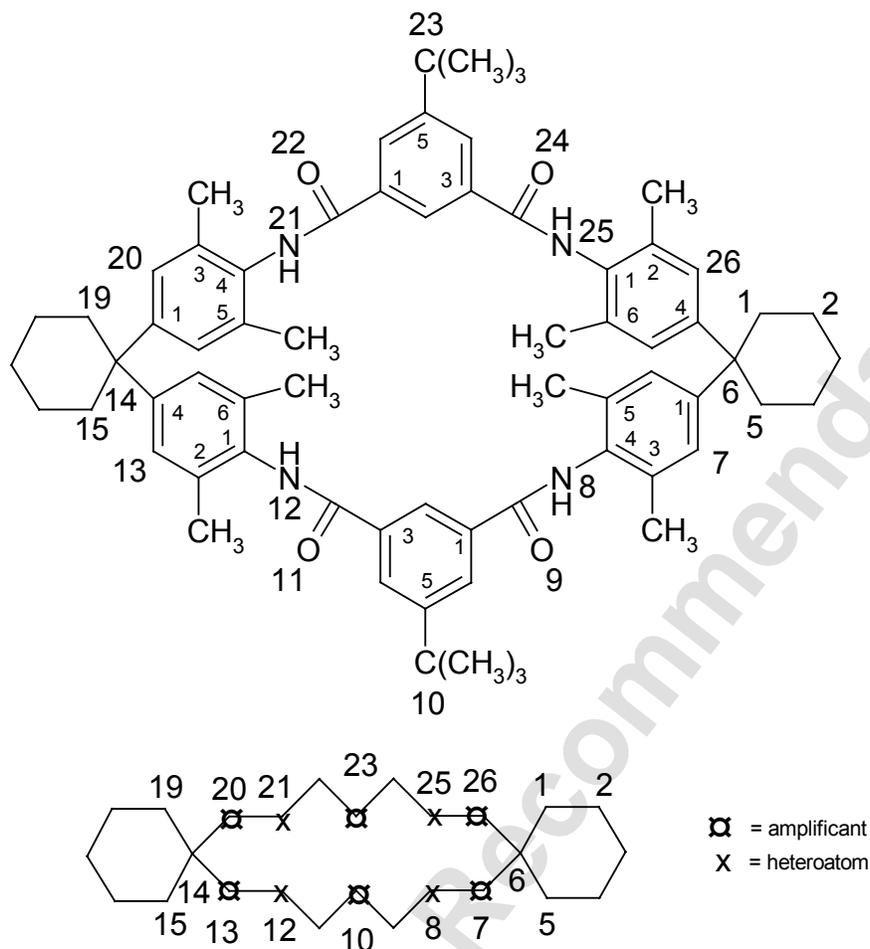


R = -OH; R' = -C(CH<sub>3</sub>)<sub>3</sub>

1<sup>5</sup>,11<sup>5</sup>,13<sup>5</sup>,16<sup>5</sup>-tetra-*tert*-butyl-13<sup>2</sup>,16<sup>2</sup>-dihydroxy-2,5,7,10-tetraoxa-6(1,8)-anthracena-1,11(2,1,3)-dibenzena-13,16(1,3)-dibenzenabicyclo[9.3.3]heptadecaphane-6<sup>9</sup>,6<sup>10</sup>-dione  
 (for the nomenclature of quinones, see ref. 2p)

R = -CH<sub>2</sub>-COO-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>3</sub> R' = -C(CH<sub>3</sub>)<sub>3</sub>

dipropyl 2,2'-[1<sup>5</sup>,11<sup>5</sup>,13<sup>5</sup>,16<sup>5</sup>-tetra-*tert*-butyl-6<sup>9</sup>,6<sup>10</sup>-dioxo-6<sup>9</sup>,6<sup>10</sup>-dihydro-2,5,7,10-tetraoxa-6(1,8)-anthracena-1,11(2,1,3)-dibenzena-13,16(1,3)-dibenzenabicyclo[9.3.3]heptadecaphane-13<sup>2</sup>,16<sup>2</sup>-diyl]diacetate



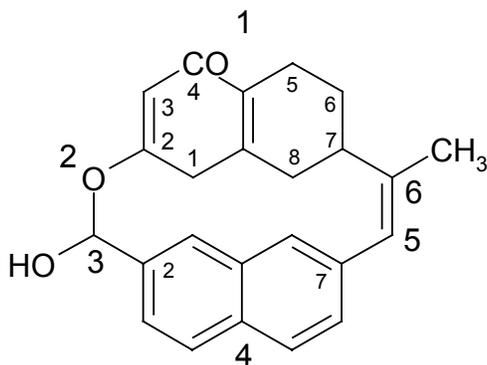
10<sup>5</sup>,23<sup>5</sup>-di-*tert*-butyl-7<sup>3</sup>,7<sup>5</sup>,13<sup>2</sup>,13<sup>6</sup>,20<sup>3</sup>,20<sup>5</sup>,26<sup>2</sup>,26<sup>6</sup>-octamethyl-8,12,21,25-tetraaza-7,13,20,26(1,4),10,23(1,3)-hexabenzendispiro[5.7.5.7]hexacosaphane-9,11,22,24-tetrone

### PhII-6.2 Writing names of polysubstituted phane derivatives

Name components are cited in the following order, from left to right:

- (1) detachable prefixes (alphabetized);
- (2) nondetachable hydro/dehydro prefixes;
- (3) nondetachable replacement 'a' prefixes;
- (4) parent hydride name;
- (5) '-ene' and '-yne' endings;
- (6) suffixes.

Example:



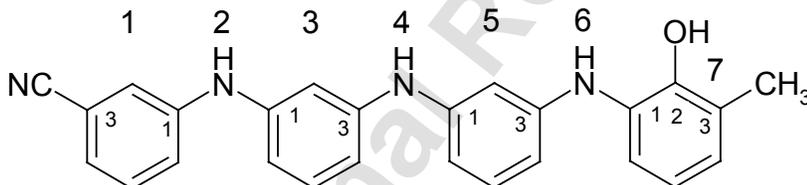
3-hydroxy-6-methyl-1<sup>5,16,17,18</sup>-tetrahydro-2-oxa-1,4(2,7)-dinaphthalenacyclohexaphan-5-en-1<sup>4</sup>(1<sup>H</sup>)-one (added hydrogen method, see PhII-3.2)

3-hydroxy-6-methyl-1<sup>1,14,15,16,17,18</sup>-hexahydro-2-oxa-1,4(2,7)-dinaphthalenacyclohexaphan-5-en-1<sup>4</sup>-one (by using the nondetachable hydro prefix, see PhII-3.2)

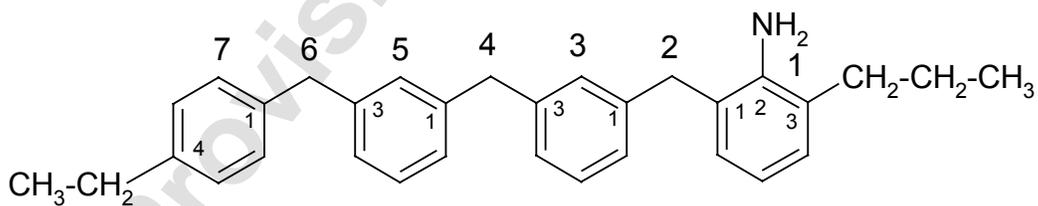
**PhII-6.3** When necessary, lowest locants are attributed to the following structural features considered successively in the order listed until a decision is reached (see PhII.1.1):

- (a) principal group named as suffix;
- (b) unsaturation (-ene/-yne endings);
- (c) substituents named as prefixes.

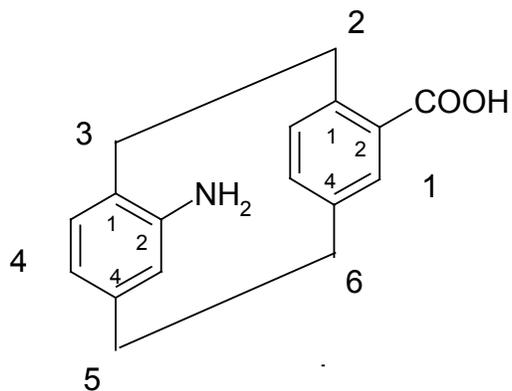
Examples:



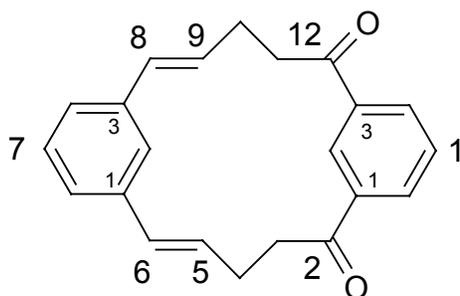
7<sup>2</sup>-hydroxy-7<sup>3</sup>-methyl-2,4,6-triaza-1,7(1),3,5(1,3)-tetrabenzenaheptaphane-1<sup>3</sup>-carbonitrile



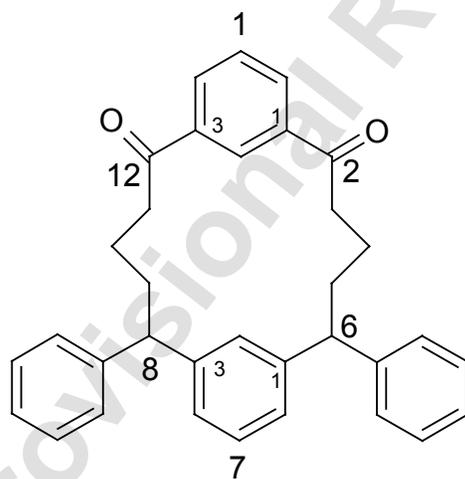
7<sup>4</sup>-ethyl-1<sup>3</sup>-propyl-1,7(1),3,5(1,3)-tetrabenzenaheptaphan-1<sup>2</sup>-amine



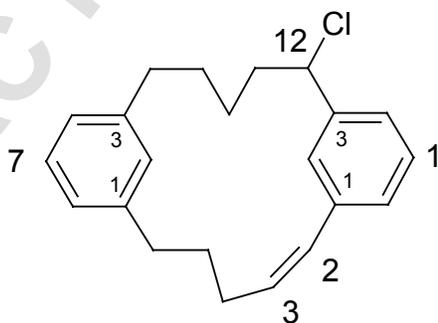
4<sup>2</sup>-amino-1,4(1,4)-dibenzenacyclohexaphane-1<sup>2</sup>-carboxylic acid



1,7(1,3)-dibenzenacyclododecaphane-5,8-diene-2,12-dione



6,8-diphenyl-1,7(1,3)dibenzenacyclododecaphane-2,12-dione



12-chloro-1,7(1,3)-dibenzenacyclododecaphan-2-ene

## References

1. International Union of Pure and Applied Chemistry. Organic Chemistry Division. Commission on Nomenclature of Organic Chemistry. Phane Nomenclature, Part I: Phane Parent Names (IUPAC Recommendations 1998). *Pure & Appl. Chem.* **70**, 1513-1545. See also IUPAC chemical nomenclature data base <<http://www.chem.qmw.ac.uk/iupac/>>. (a) PhI-2.2, pp. 1522-1523; (b) PhI-3.3, pp. 1534-1536.
2. International Union of Pure and Applied Chemistry. Organic Chemistry Division. Commission on Nomenclature of Organic Chemistry. *A Guide to IUPAC Nomenclature of Organic Compounds, Recommendations 1993*, R. Panico, W. H. Powell and J.-C. Richer, eds. Oxford: Blackwell Scientific Publications, 1993. (a) R-4.1, pp. 68-75; (b) R-5.7.4.2, pp. 117-119; (c) R-5.7.7, pp. 123-125; (d) R-5.7.6, pp. 122-123; (e) R-4.1, p. 72; (f) R-0.1.8, pp. 10-11; (g) R-0.2.4.2, p. 17; (h) R-1.3, pp. 34-35; (i) R-2.5, pp. 56-58; (j) R-0.1.8.3, pp. 10-12; (k) R-3.1.2, pp. 60-61; (m) R-3.1.3, p. 61; (n) R-3.1.1, pp. 59-60; (o) Table 10 p. 70; (p) R-5.6.2.1.
3. International Union of Pure and Applied Chemistry. Organic Chemistry Division. Commission on Nomenclature of Organic Chemistry. Revised Nomenclature for Radicals, Ions, Radical Ions and Related Species. *Pure & Appl. Chem.* **65**, pp. 1357-1455, 1993. See also IUPAC chemical nomenclature data base <<http://www.chem.qmw.ac.uk/iupac/>>. (a) RC-82.4, pp. 1411-1413.
4. International Union of Pure and Applied Chemistry. Organic Chemistry Division. Commission on Nomenclature of Organic Chemistry. Nomenclature of Fused and Bridged Fused Ring Systems. *Pure & Appl. Chem.* **70**, 143-216, 1998. See also IUPAC chemical nomenclature data base <<http://www.chem.qmw.ac.uk/iupac/>>.

01-06-04