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PHANE NOMENCLATURE. PART II. MODIFICATION OF THE DEGREE OF HYDROGENATION AND SUBSTITUTION DERIVATIVES OF PHANE PARENT HYDRIDES

(IUPAC Recommendations 2002)

Prepared for publication by
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Phane nomenclature. Part II. Modification of the degree of hydrogenation and substitution derivatives of phane parent hydrides

(IUPAC Recommendations 2002)

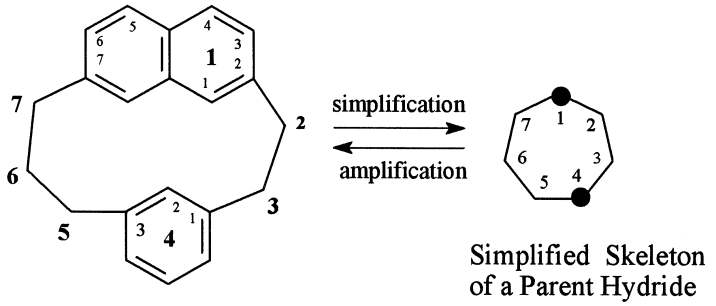
Abstract: Cyclophane and linear phane systems are considered as parent hydrides. Their derivatives are named in conformity with the principles, rules, and conventions prescribed for naming organic compounds. The following nomenclatural features are described: indicated and added hydrogen, order of seniority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

CONTENTS

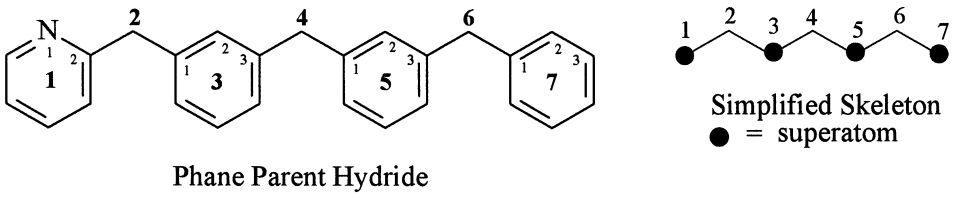
INTRODUCTION

Phane nomenclature is a new method for building names for organic structures by assembling names that describe component parts of a complex structure [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).

Examples:



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



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

The multiatomic structure is a fully saturated or mancude ring or ring system. A mancude ring or ring systems contains the maximum number of noncumulative double bonds [2]. 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 [1a]. 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.

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 [1] 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 [3a]. 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 [3b], anhydrides [3c], and acid halides [3d].

PhII-1. NUMBERING

PhII-1.1 Starting point and direction of numbering

Insofar as the general rules of substitutive nomenclature leave a choice, the starting point and direction of numbering of a compound to be named by phane nomenclature are chosen so that lowest locants are given to the following structural features, if present, considered successively in the order listed until a decision is reached [3e].

1. numbering of phane parent hydride
2. heteroatoms introduced by skeletal replacement ('a') nomenclature
3. indicated hydrogen
4. nondetachable 'hydro-'/'dehydro-' prefixes
5. principal characteristic group (named as suffix)
6. unsaturation ('-ene'/'-yne' endings and 'hydro-'/'dehydro-' prefixes)
7. substituents named as prefixes (alphabetized substituents)

PhII-1.2 'Hydro-' and 'dehydro-' prefixes

In these recommendations, 'hydro-' and 'dehydro-' prefixes are classified as nondetachable [3f]. 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 skeletal replacement ('a') prefixes, when present.

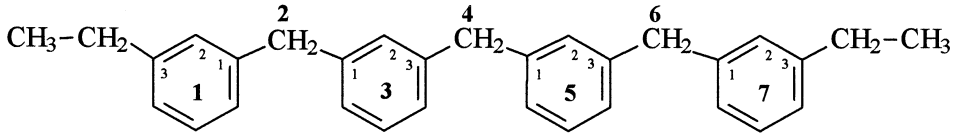
PhII-1.3 Lowest locants

When there is a choice, the established procedure for lowest locants is applied. The lowest locant set [3g] 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 alphanumerical value.

PhII-1.4 Termination of acyclic phane parent hydrides

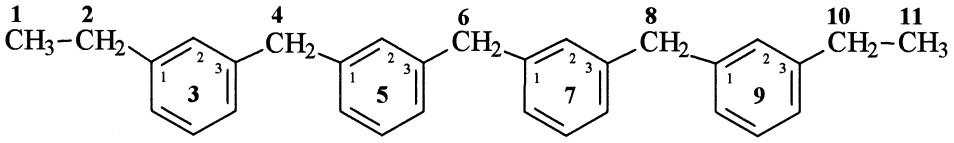
Acyclic phane parent hydrides are, by definition, terminated by an amplificant at each end of the acyclic phane system. Alkyl substituents on these terminal amplificants do not extend the phane system beyond the terminal amplificants. Names are constructed in conformity with Section PhI-3.3 [1b].

Examples:



$1^3,7^3$-diethyl-1,7(1),3,5(1,3)-tetrabenzenaheptaphane

and not

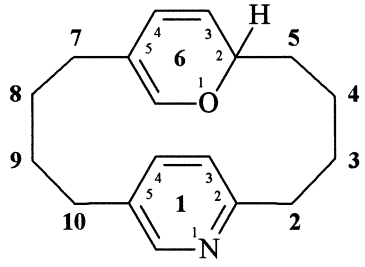


3,5,7,9(1,3)-tetrabenzenaundecaphane

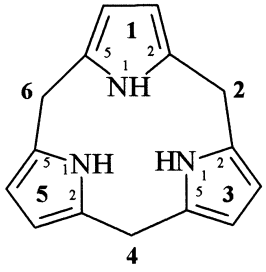
PhII-2. SPECIFICATION OF INDICATED HYDROGEN

Indicated hydrogen, when present in an amplificant, is placed before the phane parent hydride name and preceded by appropriate locants [3h].

Examples:



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



$1^1H,3^1H,5^1H$-1,3,5(2,5)tripyrrolacyclohexaphane

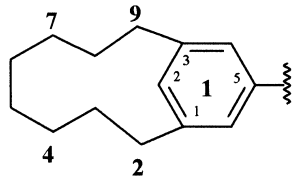
PhII-3. SUBSTITUENT GROUPS DERIVED FROM PHANE PARENT HYDRIDES

PhII-3.1 General method

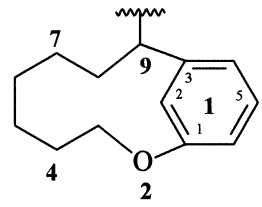
Names of substituent groups derived from phane parent hydrides are formed in accordance with the general methods [3i]. The suffixes '-yl', and '-ylidene' are added to the name of the phane parent

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'.

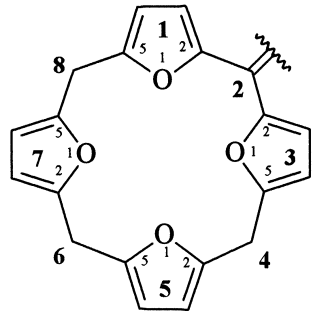
Examples:



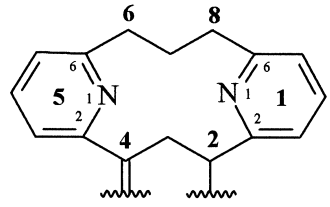
1(1,3)-benzenacyclononaphan-1^5-yl



2-oxa-1(1,3)-benzenacyclononaphan-9-yl



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

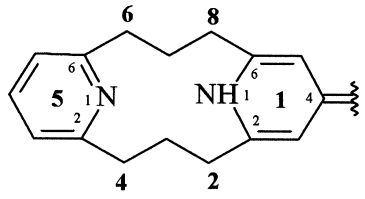


1,5(2,6)-dipyridinacyclooctaphan-2-yl-4-ylidene

PhII-3.2 'Added hydrogen' method

The 'added hydrogen' method is applied when '-ylidene' free valences are attached to a mancude ring or ring system [3h]. The method called 'added hydrogen' describes hydrogen atoms added to a specific structure as a consequence of the addition of a suffix describing a structural modification. 'Added hydrogen' is cited in parentheses after the locant describing the suffix. This type of substituent group may also be named by using nondetachable 'hydro-' prefixes [3f].

Example:



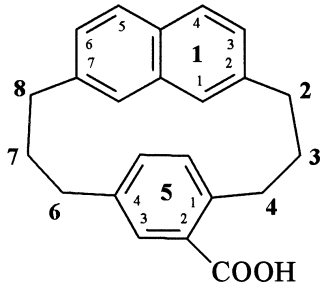
1,5(2,6)-dipyridinacyclooctaphan-1^4(1^1H)-ylidene ('added hydrogen' method)
1^1,1^4-dihydro-1,5(2,6)-dipyridinacyclooctaphan-1^4-ylidene (nondetachable 'hydro-' prefix method)

PhII-4. SUBSTITUTIVE NOMENCLATURE FOR PHANE PARENT HYDRIDES

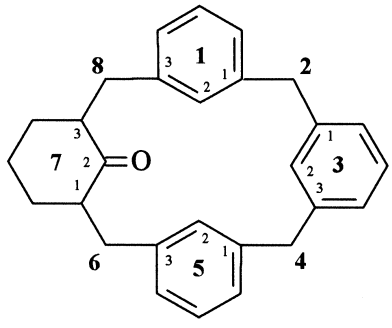
PhII-4.1 Phane parent hydrides with characteristic group suffixes

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 Section PhII-1.1).

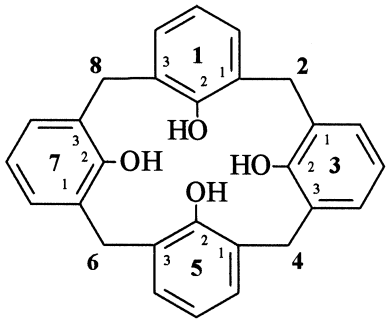
Examples:



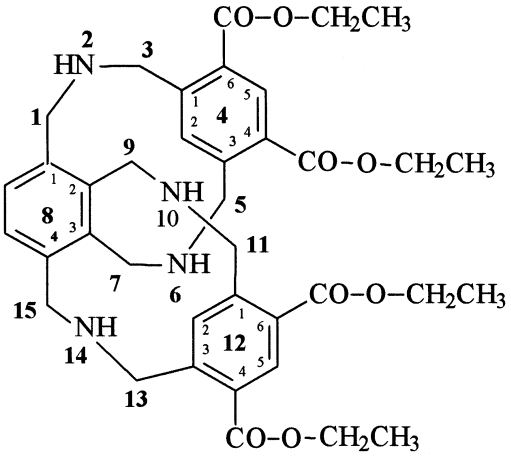
1(2,7)-naphthalena-5(1,4)-benzenacyclooctaphane-5^2-carboxylic acid

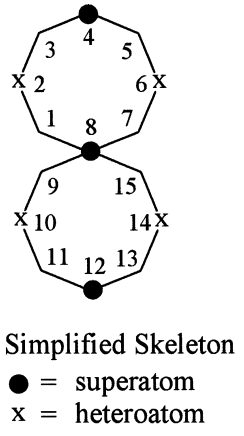


1,3,5(1,3)tribenzena-7(1,3)-cyclohexanacyclooctaphan-7^2-one

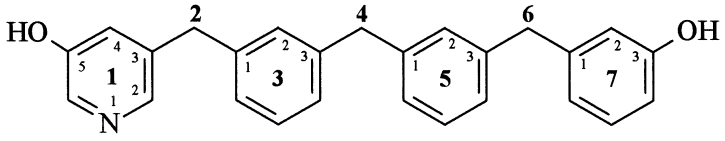


1,3,5,7(1,3)-tetrabenzenacyclooctaphane-1^2,3^2,5^2,7^2-tetrol

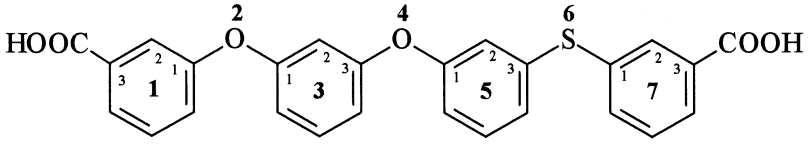




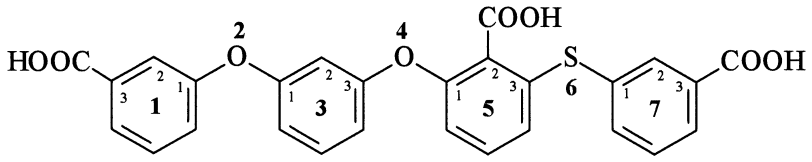
tetraethyl 2,6,10,14-tetraaza-4,12(1,3),8(1,3,2,4)-tribenzenaspiro[7.7]pentadecaphane-4^4,4^6,12^4,12^6-tetracarboxylate



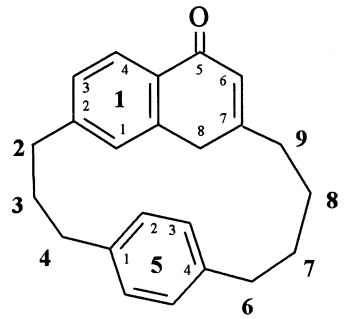
1(3)-pyridina-3,5(1,3),7(1)-tribenzenaheptaphane-1^5,$7^{\ 3}$-diol



2,4-dioxa-6-thia-1,7(1),3,5(1,3)-tetrabenzenaheptaphane-1^3,7^3-dicarboxylic acid



2,4-dioxa-6-thia-1,7(1),3,5(1,3)-tetrabenzenaheptaphane-1^3,5^2,7^3-tricarboxylic acid

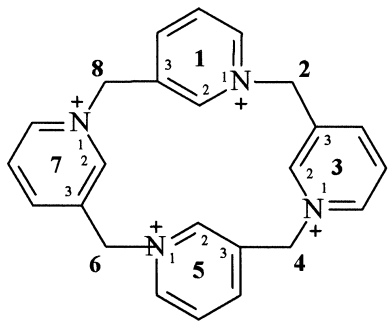


1(2,7)-naphthalena-5(1,4)-benzenacyclononaphane-1^5(1^8H)-one (added hydrogen method)
1^5,1^8-dihydro-1(2,7)-naphthalena-5(1,4)-benzenacyclononaphan-1^5-one (nondetachable 'hydro-' prefix method)

PhII-4.2 Radicals and ions derived from phane parent hydrides

Radicals are named in the same way as substituent groups (see Section PhII-3). Ions may be named by use of ionic suffixes or by using ionic replacement ('a') prefixes; ionic suffixes, such as '-ylium', are preferred over the use of skeletal replacement ('a') prefixes [4a].

Example:



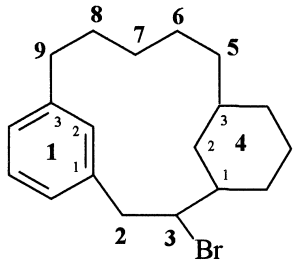
$1^1\lambda^5$,$3^1\lambda^5$,$5^1\lambda^5$,$7^1\lambda^5$-1(1,3),3,5,7(3,1)-tetrapyridinacyclooctaphane-1^1,3^1,5^1,7^1-tetrakis(ylium) (preferred)
1^1,3^3,5^3,7^3-tetraazonia-1,3,5,7(1,3)-tetrabenzenacyclooctaphane (numbering for this skeletal replacement name is based on the phane parent hydrocarbon)

PhII-4.3 Substituents of phane parent hydrides cited as prefixes

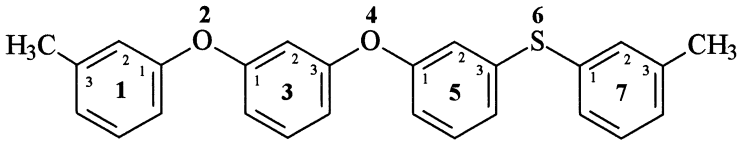
PhII-4.3.1

Atoms and/or groups cited as detachable alphabetized prefixes are assigned positions according to the fixed numbering of the phane parent hydrocarbon or the phane parent hydrocarbons modified by skeletal replacement ('a') nomenclature [3j].

Examples:



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



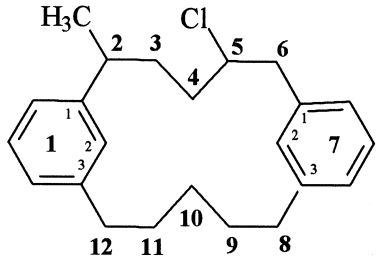
1^3,7^3-dimethyl-2,4-dioxa-6-thia-1,7(1),3,5(1,3)-tetrabenzenaheptaphane

PhII-4.3.2

When, after application of PhII-4.3.1, a choice for low locants is necessary, the following criteria are considered in order until a decision can be made.

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

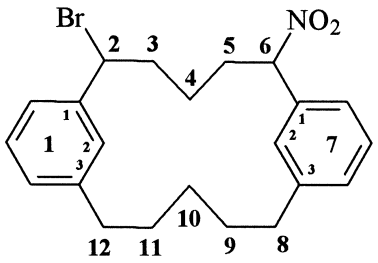
Example:



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

b. Low locants are allocated in the order of citation in the name.

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 saturated and mancude components (i.e., amplificants), and alternating chains. A mancude component has the maximum number of noncumulative double bonds. 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-' [3k] to indicate the addition of hydrogen atoms; the prefix 'dehydro-' to indicate the removal of hydrogen atoms [3m]; and the endings '-ene' and '-yne' [3n] to denote the subtraction of hydrogen atoms. The rule of lowest locants is always applied, as indicated below for specific cases.

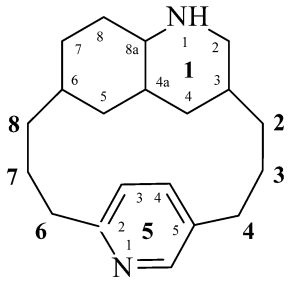
The following rules are applied, in the order given, until a decision is reached.

PhII-5.1 'Hydro-' prefixes

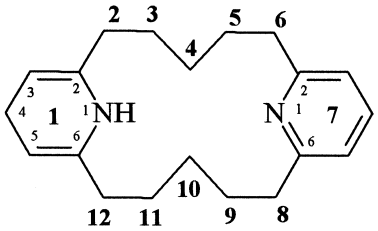
When the name of an amplificant implies the presence of the maximum number of noncumulative double bonds, other states of hydrogenation can be indicated by use of the prefix 'hydro-' together with an appropriate numerical prefix, signifying the addition of hydrogen atoms. This operation is regarded as the reduction of double bonds. Thus, hydrogen atoms can only be added in pairs, which are indicated by use of the numerical prefixes 'di-', 'tetra-', and 'hexa-' cited before the prefix 'hydro-' [3k]. Indicated hydrogen, if required by the parent hydride, is cited in front of the name of the phane parent hydride (see Section PhII-2). This method is applied as follows:

- 'Hydro-' prefixes are used to modify mancude heteromonocycles having retained names or named in accordance with the extended Hantzsch–Widman system (see ref. 3k). However, names for the corresponding fully saturated heteromonocycles that have retained names or Hantzsch–Widman names are preferred to those expressed by 'hydro-' prefixes, for example, oxolane and piperidine are preferred to tetrahydrofuran and hexahydropyridine, respectively [1a].
- 'Hydro-' prefixes are used to indicate all modifications of the degree of unsaturation of carbocyclic or heterocyclic mancude parent hydrides, except for benzene. Retained names of partially hydrogenated parent hydrides, such as indane, chromane, isochromane, pyrroline, indoline, and isoindoline, are not recommended as amplificants in phane nomenclature [1a].

Examples:



$1^{1},1^{2},1^{3},1^{4},1^{4a},1^{5},1^{6},1^{7},1^{8},1^{8a}$-decahydro-1(3,6)quinolina-5(5,2)-pyridinacyclooctaphane

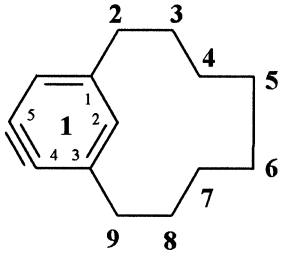


$1^{1},1^{4}$-dihydro-1,7(2,6)-dipyridinacyclododecaphane

PhII-5.2 'Dehydro-' prefixes

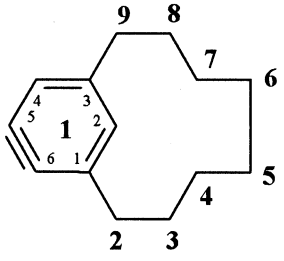
'Dehydro-' prefixes are used to indicate the removal of two contiguous hydrogen atoms from a mancude amplificant of a phane parent hydride system [3m].

Example:



$1^{4},1^{5}$-didehydro-1(1,3)-benzenacyclononaphane

not



$1^{5},1^{6}$-didehydro-1(1,3)-benzenacyclononaphane

PhII-5.3 Ene and yne endings

PhII-5.3.1 Double and triple bonds

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 site [3n].

In phane nomenclature, the endings '-ene' and '-yne' are used to denote the presence of double and triple bonds in amplificants named as saturated rings or ring systems and in simplified parent skeletons.

Note: 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' of the 'phane' ending before the vowels 'e' and 'y'.

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' and '-yne', as required.

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

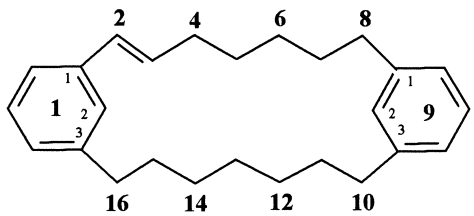
- primary locants, i.e., locants that denote the atoms and superatoms of the phane parent skeleton; in the structures herein they are the locants expressed by boldfaced arabic numbers [1b]
- composite locants, i.e., primary locants with a superscript locant denoting the positions in amplificants; expressed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

In phane nomenclature, double bonds are denoted in two ways:

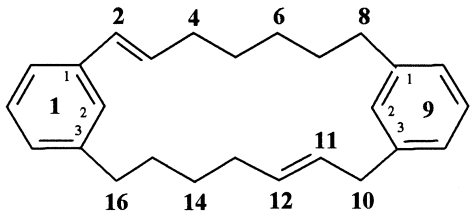
- by the lowest locant assigned to a double bond when two consecutive locants are (a) primary locants; or (b) composite locants, neither of which is adjacent to a primary locant
- by a compound locant when one locant is a composite locant adjacent to a primary locant.

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

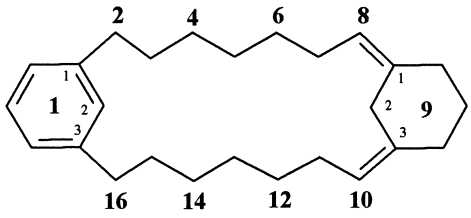
Examples:



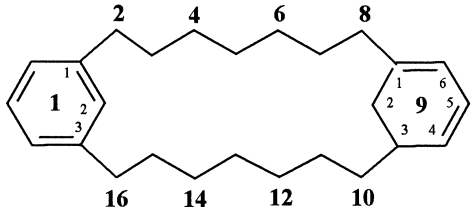
1,9(1,3)-dibenzenacyclohexadecaphan-2-ene (the numeral '2' is a primary locant)



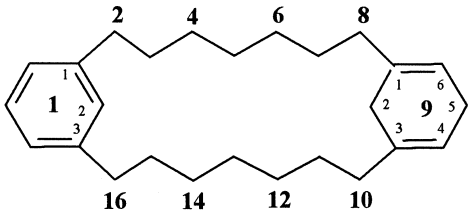
1,9(1,3)-dibenzenacyclohexadecaphane-2,11-diene (the numerals '2' and '11' are primary locants)



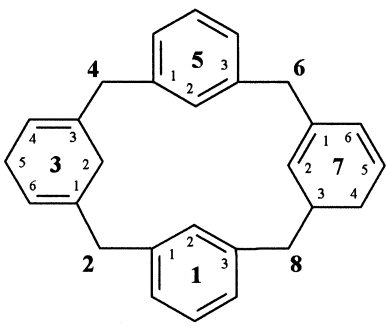
1(1,3)-benzena-9(1,3)-cyclohexanacyclohexadecaphane-8(9^1),9^3(l0)-diene [the superscripted numerals '9^1 and 9^3' are composite locants; '8(9^1) and 9^3(l0)' are compound locants; compound locants are necessary to locate precisely the position of the double bonds]



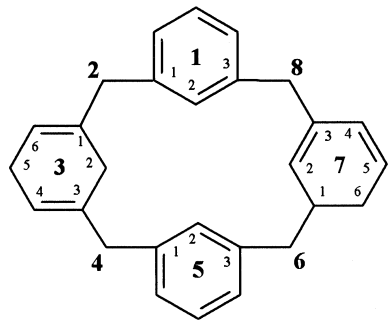
1(1,3)-benzena-9(1,3)-cyclohexanacyclohexadecaphane-9^1(9^6),9^4-diene



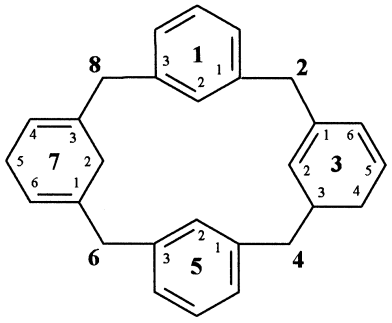
1(1,3)-benzena-9(1,3)-cyclohexanacyclohexadecaphane-9^1(9^6),9^3(9^4)-diene



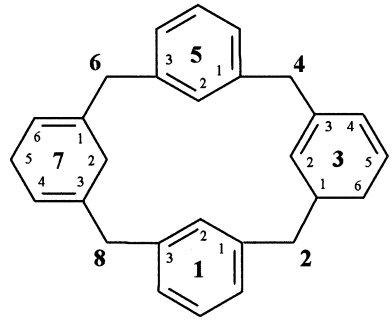
A (correct numbering)



B (incorrect numbering)



C (incorrect numbering)



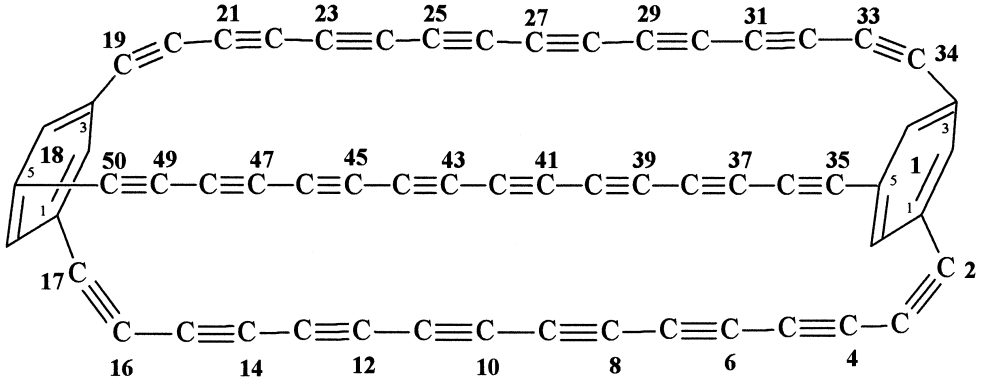
D (incorrect numbering)

1,5(1,3)-dibenzena-3,7(1,3)-dicyclohexanacyclooctaphane-$3^1(3^6),3^3(3^4),7^1(7^2),7^5$-tetraene (**A**).
[not 1,5(1,3)-dibenzena-3,7(1,3)-dicyclohexanacyclooctaphane-$3^1(3^6),3^3(3^4),7^2(7^3),7^4$-tetraene (**B**); nor 1,5(1,3)-dibenzena-3,7(1,3)-dicyclohexanacyclooctaphane-$3^1(3^2),3^5,7^1(7^6),7^3(7^4)$-tetraene (**C**); nor 1,5(1,3)-dibenzena-3,7(1,3)-dicyclo-hexanacyclooctaphane-$3^2(3^3),3^4,7^1(7^6),7^3(7^4)$-tetraene (**D**)]
[The primary locant set '3,3,7,7' for all names are identical, but the set of composite locants '$3^1,3^3,7^1,7^5$' in name **(A)**, ignoring the locant in parentheses, is lower than the locant sets '$3^1,3^3,7^2,7^4$' in (**B**), '$3^1,3^5,7^1,7^3$' in (**C**), or '$3^2,3^4,7^1,7^3$' in (**D**).]

PhII-5.3.3 Triple bonds

Triple bonds in phane nomenclature are expressed by the ending '-yne'. Triple bonds located in interconnecting chains are denoted by primary locants [3n]. If an amplificant would include one or more triple bonds, such as might be found in a large ring, composite locants, and compound locants, if required, would be necessary. Low locants are assigned to triple bonds, in the same way that as for double bonds.

Example:

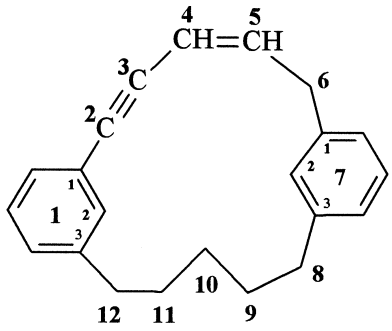


1,18(1,3,5)-dibenzenabicyclo[16.16.16]pentacontaphane-2,4,6,8,10,12,14,16,19,21,-23,25,27,29,31,33,35,37,39,41,43,45,47,49-tetracosayne

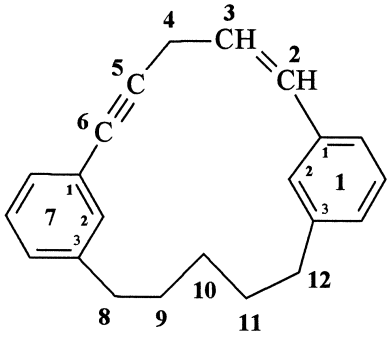
PhII-5.3.4 Double and triple bonds in a phane structure

Low locants are allocated to double and triple bonds first when considered together as a set in ascending order and, if a choice is still needed, to double bonds [3n].

Examples:

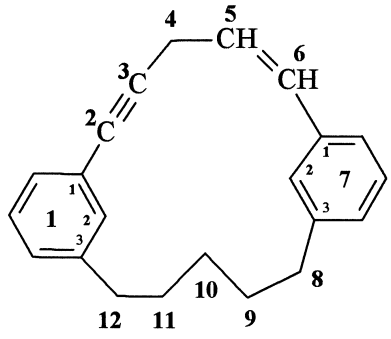


1,7(1,3)-dibenzenacyclododecaphan-4-en-2-yne



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

not

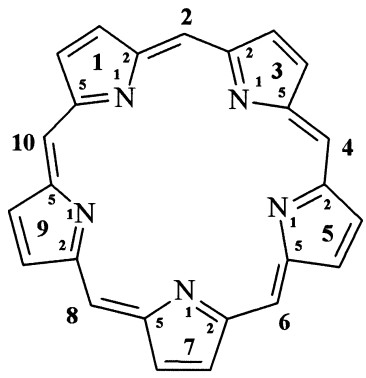


1,7(1,3)-dibenzenacyclododecaphan-5-en-2-yne

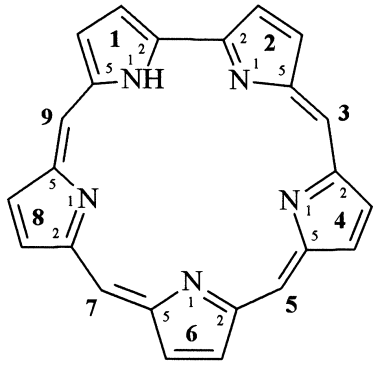
PhII-5.4 Double bonds between mancude amplificants and alternating atoms or chains

Double bonds between mancude amplificants having indicated hydrogen atoms and alternating atoms or chains are denoted by '-ene' endings. Any remaining hydrogen atoms of the mancude amplificant are cited as 'indicated hydrogen' in front of the name and take precedence for low locants over '-ene' endings. This procedure also applies to double bonds between contiguous amplificants.

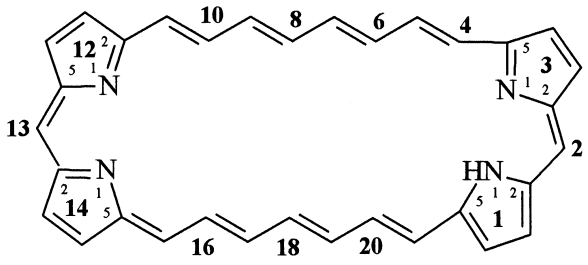
Examples:



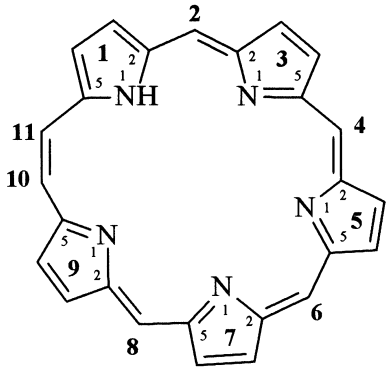
1,3,5,7,9(2,5)-pentapyrrolacyclodecaphane-1^{2}(2),3^{5}(4),5^{5}(6),7^{5}(8),9^{5}(10)-pentaene



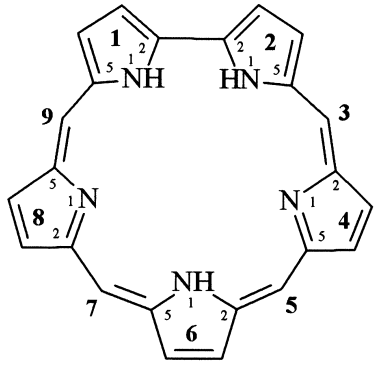
1^{1}*H*-1,2,4,6,8(2,5)-pentapyrrolacyclononaphane-2^{5}(3),4^{5}(5),6^{5}(7),8^{5}(9)-tetraene



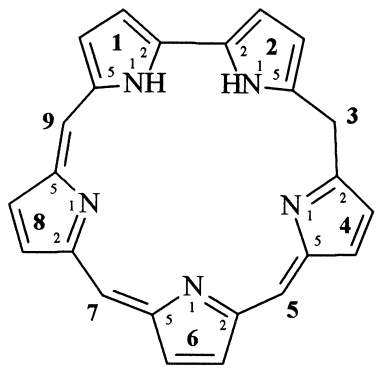
1^{1}*H*-1,3,12,14(2,5)-tetrapyrrolacyclohenicosaphane-2(3^{2}),4,6,8,10,12^{5}(13),14^{5}(15),16,18,20-decaene



1^{1}*H*-1,3,5,7,9(2,5)-pentapyrrolacycloundecaphane-2(3^{2}),4(5^{2}),6(7^{2}),8(9^{2}),10-pentaene



$1^1H,2^1H,6^1H$-1,2,4,6,8(2,5)-pentapyrrolacyclononaphane-3(4^2),5(6^2),6^5(7),8^5(9)-tetraene [The trivial name for this pentapyrrolic macrocycle is sapphyrin (see ref. 5 for the numbering of this structure following the system for cyclic tetrapyrroles).]



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

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

When double bonds are located between partially or fully hydrogenated mancude amplificants and acyclic components of a phane structure, double bonds are denoted by the ending '-ene' and the hydrogenation of the mancude amplificant is indicated by the usual prefix 'hydro-'. Names can be formed by the following two methods, method (a) being preferred.

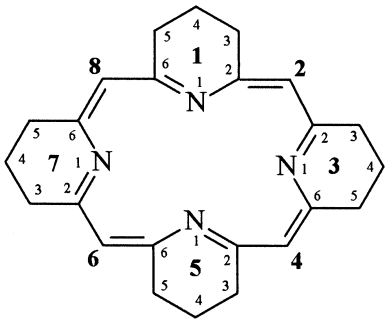
For **method (a)** the order of operations is as follows:

1. insert the double bonds indicated by '-ene' endings;
2. add the maximum number of double bonds in the amplificant rings;
3. cite indicated hydrogen atoms, in accordance with the numbering of the amplificant;
4. saturate the appropriate double bonds using 'hydro-' prefixes.

This method, i.e., the introduction of double bonds denoted by the '-ene' endings followed by the insertion of the maximum number of noncumulative double bonds, is analogous to the method described in FR-8.1.2 [6] for naming bridged ring systems, in which the bridge is introduced followed by the addition of the maximum number of noncumulative double bonds.

For **method (b)**, nondetachable 'hydro-' prefixes are used. Lowest locants are assigned first to indicated hydrogen, if present, then to 'hydro-' prefixes, and finally to double bonds denoted by '-ene' endings (see Section PhII-1.1).

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)-tetrapyridinacyclooctaphane-$1^2(2),3^6(4),5^6(6),7^6(8)$-tetraene

The formation of this name may be understood by referring to structures **A**, **B**, and **D**, below. The names for these structures are as follows:

A 1,3,5,7(2,6)-tetrapyridinacyclooctaphane

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

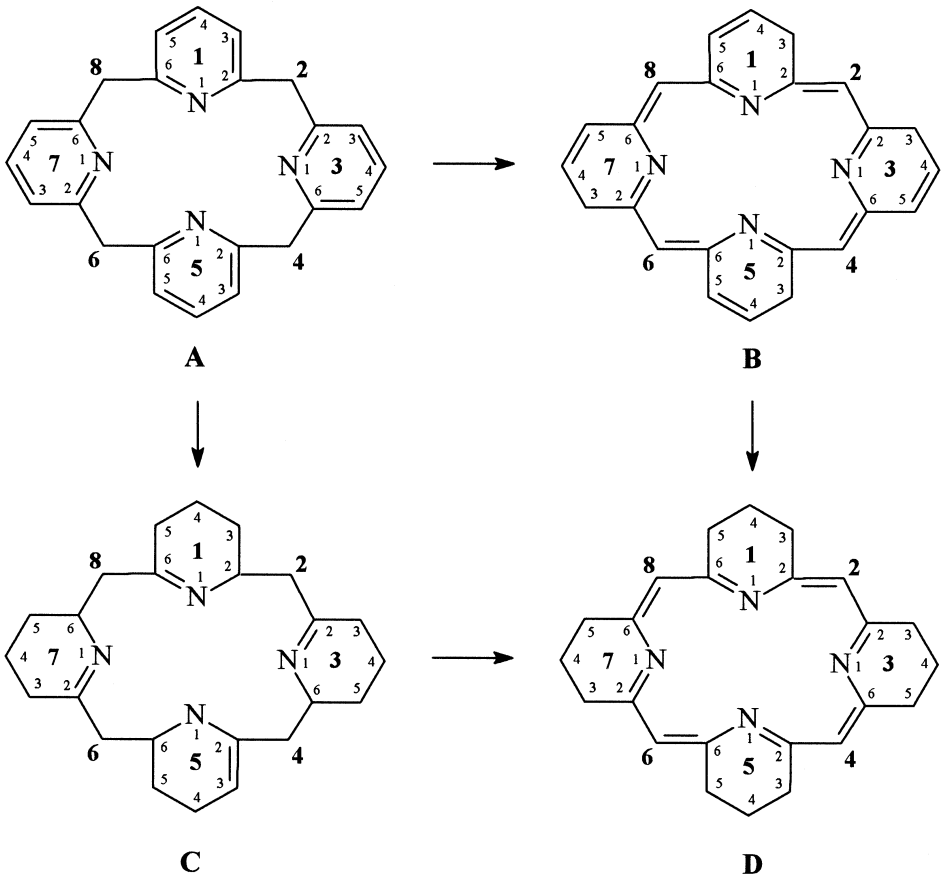
Method (b): $1^2,1^3,1^4,1^5,3^3,3^4,3^5,3^6,5^3,5^4,5^5,5^6,7^3,7^4,7^5,7^6$-hexadecahydro-1,3,5,7(2,6)-tetrapyridinacyclooctaphane-$1^2(2),3^6(4),5^6(6),7^6(8)$-tetraene

The formation of this name may be understood by referring to structures **A**, **C**, and **D**, below. The names for these structures are as follows:

A 1,3,5,7(2,6)-tetrapyridinacyclooctaphane

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)-tetrapyridinacyclooctaphane

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)-tetrapyridinacyclooctaphane-$1^2(2),3^6(4),5^6(6),7^6(8)$-tetraene

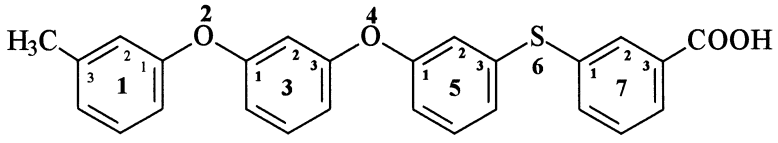


PhII-6. POLYSUBSTITUTED DERIVATIVES OF PHANE PARENT HYDRIDES

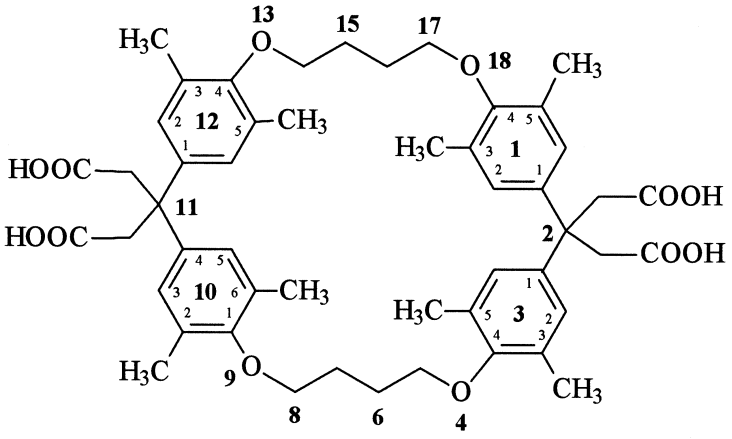
PhII-6.1 Principal characteristic groups

The order of priority of classes (see Table 10, ref. 3o) is applied to select the principal characteristic group. Characteristic groups that are not selected as the principal characteristic group are cited as prefixes. 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). Lowest locants are assigned in conformity with this fixed numbering first to the principal characteristic groups and then to groups cited as prefixes.

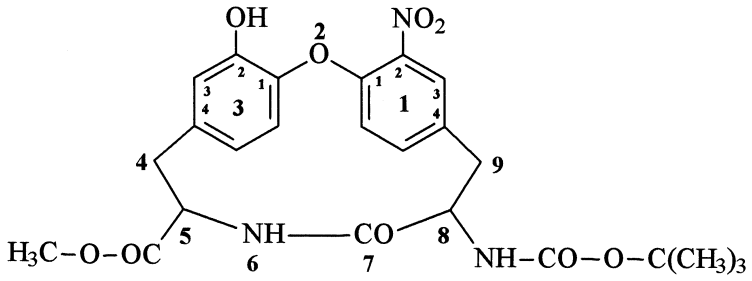
Examples:



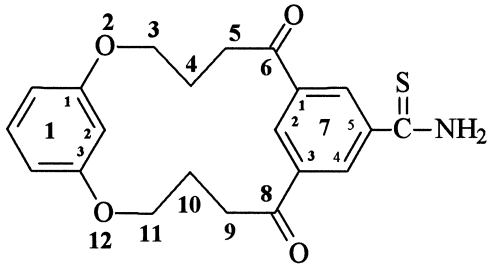
1^3-methyl-2,4-dioxa-6-thia-1,7(1),3,5(1,3)-tetrabenzenaheptaphane-7^3-carboxylic acid



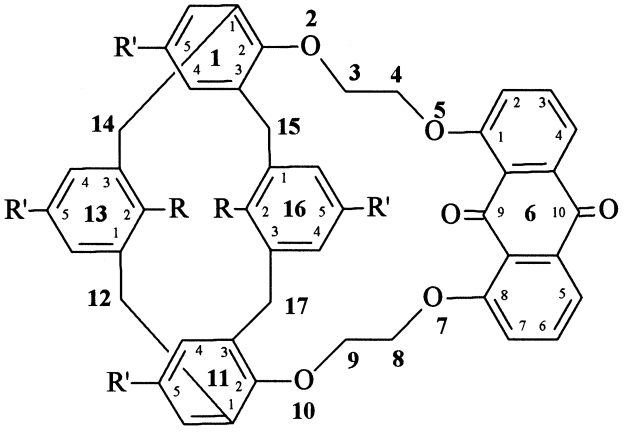
2,2′,2″,2‴-[1^3,1^5,3^3,3^5,10^2,10^6,12^3,12^5-octamethyl-4,9,13,18-tetraoxa-1,3,10,12(1,4)- tetrabenzenacyclooctadecaphane-2,2,11,11-tetrayl]tetraacetic acid

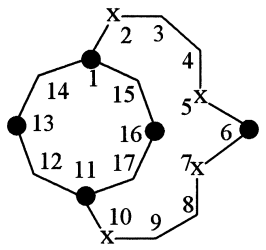


methyl 8-[(*tert*-butoxycarbonyl)amino]-3^2-hydroxy-1^2-nitro-7-oxo-2-oxa-6-aza-1,3(1,4)-dibenzenacyclononaphane-5-carboxylate



6,8-dioxo-2,12-dioxa-1,7(1,3)dibenzenacyclododecaphane-7^5-carbothioamide





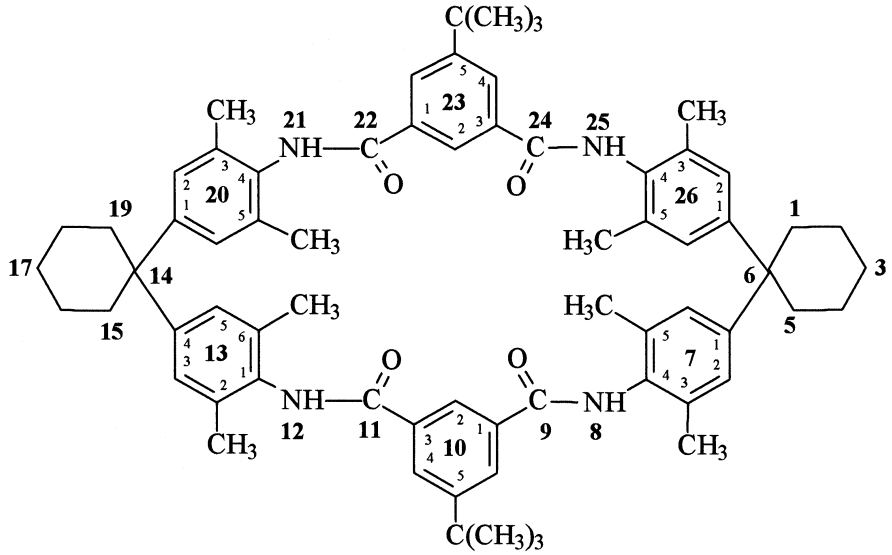
Simplified Skeleton
● = superatom
x = heteroatom

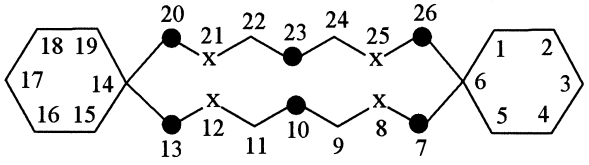
R = –OH; R′ = $–C(CH_3)_3$

$1^5,11^5,13^5,16^5$-tetra-*tert*-butyl-$13^2,16^2$-dihydroxy-2,5,7,10-tetraoxa-6(1,8)-anthracena-1,11(2,1,3),13,16(1,3)-tetrabenzenabicyclo[9.3.3]heptadecaphane-$6^9,6^{10}$-dione (for the nomenclature of quinones, see ref. 3p)

R = $–CH_2$-COO-CH_2-CH_2-CH_3; R′ = $–C(CH_3)_3$

dipropyl 2,2′-[$1^5,11^5,13^5,16^5$-tetra-*tert*-butyl-$6^9,6^{10}$-dioxo-$6^9,6^{10}$-dihydro-2,5,7,10-tetraoxa-6(1,8)-anthracena-1,11(2,1,3),13,16(1,3)-tetrabenzenabicyclo[9.3.3]heptadecaphane-$13^2,16^2$-diyl]diacetate





Simplified Skeleton
● = superatom
x = heteroatom

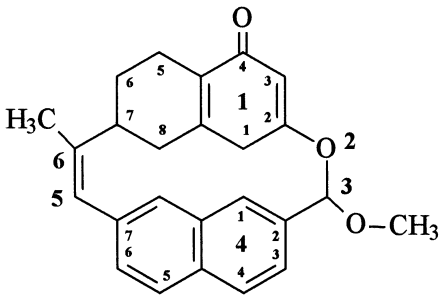
10^{5},23^{5}-di-*tert*-butyl-7^{3},7^{5},13^{2},13^{6},20^{3},20^{5},26^{3},26^{5}-octamethyl-8,12,21,25-tetraaza-7,13,20,26(1,4),10,23(1,3)-hexabenzenadispiro[5.7.5^{14}.7^{6}]hexacosaphane-9,11,22,24-tetrone

PhII-6.2 Name component order for polysubstituted phane derivatives

Writing of polysubstituted phane names follows the normal order for writing names for organic compounds. The name components for polysubstituted phane derivatives 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-methoxy-6-methyl-1^5,1^6,1^7,1^8-tetrahydro-2-oxa-1,4(2,7)-dinaphthalenacyclohexaphan-5-en-1^4(1^1*H*)-one (added hydrogen method, see Section PhII-3.2)

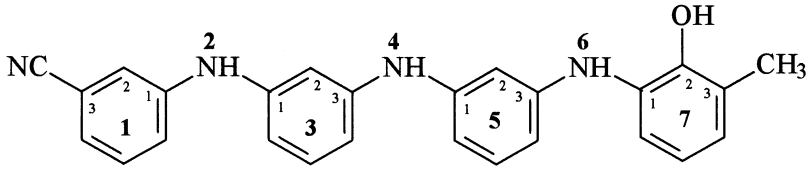
3-methoxy-6-methyl-1^1,1^4,1^5,1^6,1^7,1^8-hexahydro-2-oxa-1,4(2,7)-dinaphthalenacyclohexaphan-5-en-1^4-one (nondetachable 'hydro-' prefixes, see Section PhII-3.2)

PhII-6.3 Order for assignment of lowest locants for phane derivatives

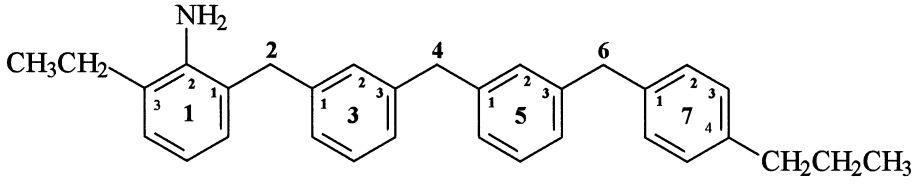
When necessary, lowest locants are attributed to the following structural features considered successively in the order listed until a decision is reached (see Section PhII-1.1):

1. principal group named as suffix;
2. unsaturation ('-ene'/'-yne' endings);
3. substituents named as prefixes:

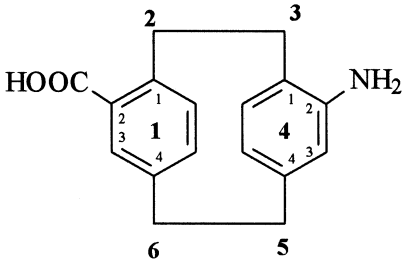
Examples:



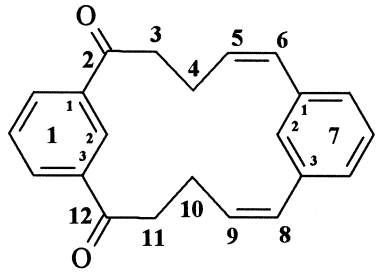
7^2-hydroxy-7^3-methyl-2,4,6-triaza-1,7(1),3,5(1,3)-tetrabenzenaheptaphane-1^3-carbonitrile



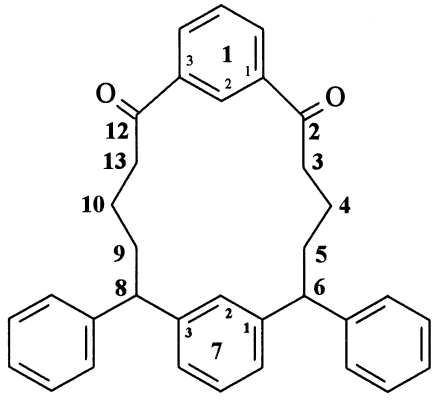
1^3-ethyl-7^4-propyl-1,7(1),3,5(1,3)-tetrabenzenaheptaphan-1^2-amine



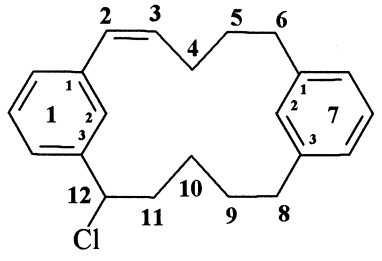
4^2-amino-1,4(1,4)-dibenzenacyclohexaphane-1^2-carboxylic acid



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

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