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ORGANIC CHEMISTRY DIVISION

COMMISSION ON NOMENCLATURE OF ORGANIC CHEMISTRY\*

**PHANE NOMENCLATURE**  
**PART I: PHANE PARENT NAMES**

(IUPAC Recommendations 1998)

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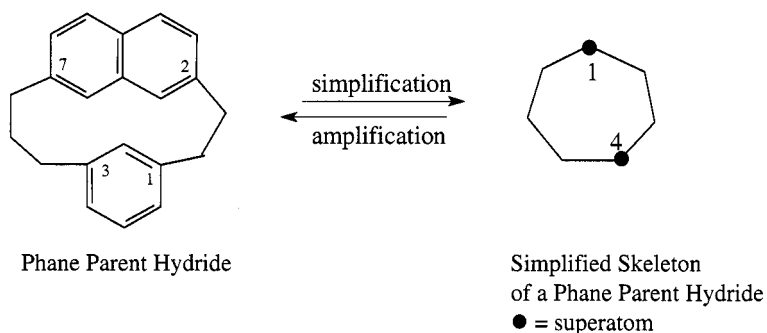
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## Phane nomenclature Part I. Phane parent names (IUPAC recommendations 1998)

*Abstract:* Phane nomenclature is a new method for building names for organic structures by assembling names that describe component parts of a complex structure. It is based on the idea that a relatively simple skeleton for a parent hydride can be modified by an operation called 'amplification', a process that replaces one or more special atoms (superatoms) of a simplified skeleton by multiatomic structures. In this set of recommendations, multiatomic structures are fully saturated rings or ring systems or unsaturated rings or ring systems with the maximum number of noncumulative double bonds (mancude). In the amplification operation each superatom is replaced by a ring or ring system identified in the name 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 the superatoms, are, by convention, traditional 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 traditional skeletal replacement ('a') prefixes, such as 'oxa', 'aza', etc., that indicate replacement of a single skeletal unit of structure, usually a carbon unit, by a different unit of structure.



Simplified skeletal name: cycloheptaphane

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

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 expressed by the amplification prefixes that are linked to the adjacent normal atoms of the simplified parent skeleton.

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

<b>CONTENTS</b>	<b>Page</b>
Preamble	1515
Introduction	1517
Recommendations	1517
PhI-1. Concepts and terminology	1517
PhI-1.1. Simplification and amplification	
PhI-1.2. Simplified skeleton of the phane parent hydride, simplified phane parent graph, simplified skeletal name, and skeletal locants	
PhI-1.3. Superatom and superatom locant	
PhI-1.4. Amplificant, amplification prefix, and amplificant locant	
PhI-1.5. Attachment atom and attachment locant	
PhI-1.6. Phane parent skeleton, phane parent name, and phane parent hydride	
PhI-2. Components of phane parent names	1519
PhI-2.1. Simplified skeletal names	
PhI-2.1.1. Unbranched acyclic simplified skeletons	
PhI-2.1.2. Monocyclic simplified skeletons	
PhI-2.1.3. Multicyclic simplified skeletons without free spiro nodes	
PhI-2.1.4. Multicyclic simplified skeletons with spiro nodes but no bridgehead nodes	
PhI-2.1.4.1. Monospiro simplified skeletons	
PhI-2.1.4.2. Linear unbranched multispiro simplified skeletons	
PhI-2.2. Amplification prefixes	
PhI-2.2.1. Parent hydride names for deriving amplification prefix names	
PhI-2.2.2. Formation of amplification prefix names	
PhI-2.2.3. Order of citation of amplification prefixes	
PhI-2.2.4. Multiple identical amplificants	
PhI-2.3. Superatom locants and amplificant attachment locants	
PhI-2.3.1. Superatom locants	
PhI-2.3.2. Attachment locants	
PhI-3. Numbering of phane parent hydrides	1525
PhI-3.1. Numbering of phane parent skeletons and amplificants	
PhI-3.2. Numbering of simplified phane skeletons with respect to amplificant numbering	
PhI-3.3. Numbering of phane parent hydrides	
PhI-4. Skeletal replacement ('a') nomenclature in phane nomenclature	1536
PhI-4.1. Name construction	
PhI-4.2. Skeletal replacement ('a') nomenclature in simplified skeletal names	
PhI-4.3. Skeletal replacement ('a') nomenclature in amplificants	
PhI-4.4. Simultaneous skeletal replacement in amplificants and simplified skeletal names	
PhI-4.5. Numbering of heterophane parent hydrides with respect to heteroatoms described by skeletal replacement ('a') nomenclature	
PhI-5. Guide to construction of phane parent hydride names	1543
References	1544

## PREAMBLE

Systematic nomenclature of organic chemistry (refs 1,2) consists of various methods for building a name for a structure by assembling names that describe composite parts of its structure. Components of a systematic name describe individual parts of the structure of an organic compound and provide details of its structure. Not only do the components imply structural information, but they also provide information

as to how a component is connected to the rest of the structure. This information is usually provided in terms of modifications to a parent structure; such modifications are called 'operations'. Different types of operations may be considered to represent steps of systematic nomenclature appropriate for different kinds of organic compounds.

Among the various types of operations, the following are important in deriving names for cyclic structures:

- (a) **ortho and ortho/peri-Fusion**, expressed by fusion prefixes, such as 'benzo' in the name 'benzo[f]quinoline';
- (b) **Spiro union or fusion**, expressed by the operational prefix 'spiro' as in the name 'spiro[piperidine-4,9'-xanthene]';
- (c) **Bridging**, expressed by bridging prefixes, such as 'methano' in the name '1,4-methanonaphthalene'.

In addition, an operation involved in naming identical cyclic structures with only one bond linking one to another is:

**Conjunctive union**, expressed by prefixes such as 'bi', 'ter', etc., as in the name '2,2'-bipyridine'.

In this publication, recommendations are given establishing another method for naming complex cyclic structures. It is based on the novel concept of reducing the complexity of a structure to a simpler ring, ring system, or even to a chain. This new method is called 'Phane Nomenclature' because of the ending 'phane' that is compulsory in all names involving the principles of this new method. Even though the term 'cyclophane' has been used to describe a particular type of cyclic structure (ref. 3), no attempt is made in this presentation to restrict 'phane' in such a sense.

The recommendations presented herein have been derived from various sources. In 1951, a proposal for describing a relatively small family of structures consisting of two or more benzene rings cyclically interconnected by carbon atoms or chains appeared (ref. 3). In the name 'cyclophane' proposed for this class of compounds, the 'ph' was derived from 'phenylene', the name for expressing the presence of a benzene ring between two separate parts of a structure. Numerical terms were used as part of these names to specify connecting positions. This idea found acceptance, and a desire soon arose to use analogous names for structures containing rings or ring systems other than benzene. Thus, it was suggested (refs 4,5) that such names be characterized by the term 'phane' and that names available for various rings and ring systems be used to indicate the presence of other rings. At this point the term 'phane' became a class name. The use of the prefix 'benzena' for denoting the replacement of a saturated atom in a cyclic structure by a phenylene group, first appeared in 1957 (ref. 6). Later, it was proposed that established hydrocarbon names be used for specification of other hydrocarbon rings (refs 7,8). Numerous amendments and extensions of this method have been proposed (refs 9–13), many of which have been incorporated into the present recommendations. By generalization and adaptation of established nomenclature techniques, the method has finally been tailored so that it is fully compatible with existing systematic nomenclature of organic chemistry.

Among the established methods of systematic nomenclature of organic chemistry, skeletal replacement ('a') nomenclature (refs 1a,2a) is well known and widely used. Its operational concept is the replacement of one skeletal atom of a structure by another atom, each with its proper complement of hydrogen atoms, as in the name '3,6,9,12-tetraoxatetradecane', in which the prefix 'oxa' in combination with the multiplicative prefix 'tetra' indicates replacement of each of four carbon atoms of the fourteen-membered carbon chain by an oxygen atom. In a phane replacement operation, a superatom of a simplified skeleton is replaced by a multiatomic (cyclic) structural unit. Thus, this new operation represents an extension of the traditional skeletal replacement technique. By this extension, this new method becomes as versatile as substitution, i.e., the exchange of one or more hydrogen atoms for a single atom or a group of atoms. Since both replacement techniques are compatible, their use together in systematic names provides an efficient means for naming complex heterocyclic structures.

## INTRODUCTION

The recommendations in this report provide the basic rules necessary to ensure generation of unique and unambiguous names based on the novel concept of phane nomenclature within the framework of the traditional systematic nomenclature for organic compounds.

**PhI-1** describes the fundamental concepts of the method by means of definitions of the terminology that will be needed for understanding the rules given in subsequent sections, PhI-2, PhI-3, and PhI-4.

**PhI-2** is divided into two subsections that provide the basic rules for formation of phane parent name components:

**PhI-2.1** the simplified skeletal name, which specifies the framework that is the parent structure for the amplification operation; and,

**PhI-2.2** the amplification prefixes, which specify the amplifiants, i.e., the cyclic parts of the original structures restored by the amplification operation.

**PhI-3** delineates the rules for unique and unambiguous numbering of simplified skeletal structures and of phane parent hydrides.

**PhI-4** gives the rules for generating heterocyclic phane parent hydride names using traditional skeletal replacement ('a') nomenclature in combination with phane nomenclature.

**PhI-5** is a guide to the construction of phane parent hydride names.

The comprehensive system needs additional rules. The rules in this report will allow the application of the usual substitution operations. Rules related to the combination of phane nomenclature with other aspects of traditional systematic nomenclature, such as modification of the degree of hydrogenation, the use of indicated and added hydrogen, and stereodescriptors needed for phane names will be given in subsequent publications.

The examples given herein to illustrate details of the method have been chosen with didactic intent. As such, they far exceed the average complexity of structures that are normally encountered; however, they do illustrate that the use of this method demands some care. Furthermore, these examples will show that this new method is more convenient than existing ones for naming highly complex cyclic structures.

In the examples of phane parent hydrides that follow, the larger bold-faced numbers are the locants of the simplified phane skeleton and the small numbers are the locants of the individual amplifiants. In the representations of simplified skeletons, superatoms are indicated by large dots and in PhI-4 the letter 'x' represents heteroatoms that are to be described by the skeletal replacement ('a') operation.

## RECOMMENDATIONS

### PhI-1. CONCEPTS AND TERMINOLOGY

Definitions of terms that will be encountered in these recommendations are given below. These terms refer to types of operations, to the components of phane names, and to details of structure involved in the operations. They clearly describe the basis of phane nomenclature.

#### PhI-1.1. Simplification and amplification

The fundamental operations of phane nomenclature are illustrated in the diagram shown in Fig. 1. The operation proceeding from left to right is called **simplification**; the reverse operation is called **amplification**, or phane replacement.

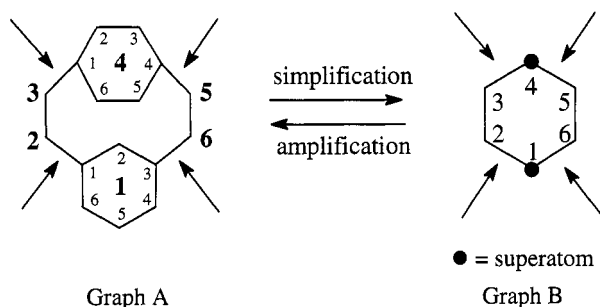


Fig. 1. Phane nomenclature conversion diagram.

The simplification operation illustrates the initial step in the process of assembling a phane parent name, i.e., nomenclaturally significant segments of a complex cyclic structure are replaced by single 'atoms' called 'superatoms' (see PhI-1.3), thus producing a simplified skeleton that can be named more easily. The phane parent hydride name (see PhI-1.6) is then formed from the names of components for the portions of structure so obtained, i.e., the 'simplified parent skeleton' provides the phane skeletal name and the names for the amplificants designate the portions of the phane parent hydride replaced by the simplification procedure. In contrast to other bonds associated with the amplificant, the bonds marked by arrows in Fig. 1 do not disappear in the simplification or amplification operations.

### PhI-1.2. Simplified skeleton of the phane parent hydride, simplified phane parent graph, simplified skeletal name, and skeletal locants

Graph B in Fig. 1 at which simplification ends and amplification starts is called the **simplified skeleton** of the phane parent hydride and is represented by a **simplified phane parent graph**. Its name is the **simplified skeletal name**. A simplified skeletal name implies a specific skeletal numbering (see PhI-2.1); its locants are **skeletal locants**, which become the primary locants for the phane parent hydride name.

### PhI-1.3. Superatom and superatom locant

The 'atoms' of the simplified skeleton shown by the enlarged dots in positions 1 and 4 of Graph B in Fig. 1 that appear on simplification and disappear on amplification are called **superatoms**. Their locants in the simplified skeleton of the parent are called **superatom locants** (see PhI-2.3.1) and are a subset of the locant set that describes the location and orientation of the amplificants (see PhI-1.4). In graph theory, 'atoms' and 'superatoms' are both nodes (or vertices). Accordingly, it can be said that the simplified phane parent graph contains both monoatomic and polyatomic nodes and is a contraction of the complete formula graph (shown as Graph A in Fig. 1). The amplificants are subgraphs of the phane parent graph.

### PhI-1.4. Amplificant, amplification prefix, and amplificant locant

A multiatomic unit of structure replacing a 'superatom' in the amplification operation is called an **amplificant**; the six-membered rings in Graph A in Fig. 1 are amplificants. They are expressed in a phane parent name (see PhI-1.6) by **amplification prefixes** (see PhI-2.2). Each such prefix implies a specific numbering of the amplificant (see also PhI-2.2.1.1); the respective locants are called **amplificant locants** and are shown as the smaller numbers in Graph A of Fig. 1.

### PhI-1.5. Attachment atom and attachment locant

The atoms of an amplificant to which the bonds marked by arrows in Fig. 1 are attached are called **attachment atoms**, and their locants are **attachment locants**. In Graph A of Fig. 1, amplificant locants

'1' and '4' are the attachment locants of the upper ring and amplificant locants '1' and '3' are the attachment locants of the lower ring (see PhI-2.3.2).

### PhI-1.6. Phane parent skeleton, phane parent name, and phane parent hydride

The skeletal graph at the start of a simplification operation or resulting from an amplification operation (see Graph A in Fig. 1) is called a **phane parent skeleton**. Correspondingly, the combination of the simplified parent name, amplification prefixes, and the appropriate superatom and attachment locants (see PhI-2.3) is called a **phane parent name**. The term 'parent' indicates that it may be combined with names for other components of the structure derived from the operations of systematic nomenclature of organic chemistry, such as substitutive prefixes, hydrogenation prefixes, and characteristic group suffixes; thus, the name becomes the parent for the various operations of traditional substitutive nomenclature. In the absence of such other components, the compound is a **phane parent hydride**, which means that the name implies the order of all bonds of the skeletal parent and thus the number of hydrogen atoms attached to each of the skeletal atoms.

## PhI-2. COMPONENTS OF PHANE PARENT NAMES

### PhI-2.1. Simplified skeletal names

A simplified skeletal name consists of the term 'phane' preceded by a name specifying the structure of the simplified parent skeleton; this name is a parent for amplification but for no other operation. The simplification operation must be done in such a way that the amplificants can be expressed by amplification prefixes that are acceptable according to PhI-2.2.1.

*Note:* It might seem desirable to form simplified skeletal names using the usual hydrocarbon names, i.e., names ending with 'ane', rather than to introduce the new ending 'phane'. However, it is important to have an ending that indicates the presence of a skeletal graph in which some nodes do not represent single atoms. Having 'phane' as a compulsory term for all names involving simplification/amplification operations ensures that in normal hydrocarbon names, such as 'hexane' or 'cyclononane', all nodes will continue to represent single carbon units.

A bond order of one is assumed for all bonds expressed by a simplified skeletal name. Atoms (nodes) not identified by amplification prefixes as 'superatoms' represent, by convention, carbon atoms with a bonding number ('valency') of four in accordance with the principles of organic nomenclature. In contrast to such carbon atoms, the bonding number of 'superatoms' is unlimited; they never have bonds other than their skeletal bonds.

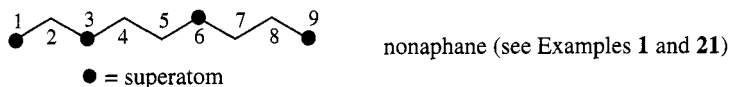
*Note:* In a phane parent hydride, therefore, the bonding number ('valency') of a 'superatom' always equals the number of bonds connecting it to neighboring atoms of the simplified skeleton, which is clear from the phane parent name. Accordingly, since the bonding number of a superatom is unlimited, there will be simplified skeletons for which a corresponding hydrocarbon structure is not possible. In order to name such skeletons, extension of the long established principles for naming hydrocarbons in systematic nomenclature is needed. These extensions will be described in a forthcoming publication.

Superatoms of a simplified skeletal name are assigned the lowest locant or the lowest set of locants, consistent with the numbering of the skeletal class to which it belongs. The lowest set of locants is the one that has the locant with the lowest numerical value at the first point of difference when the sets are compared term by term in order of increasing value (refs 1b,2b).

#### PhI-2.1.1 Unbranched acyclic simplified skeletons

The name of an unbranched acyclic simplified parent skeleton consists of a numerical term, 'tri', 'tetra', etc., indicating the number of nodes in the chain followed by the term 'phane'. The nodes of the chain are numbered consecutively from one end to the other and superatoms are given preference for low numbers.

Example:



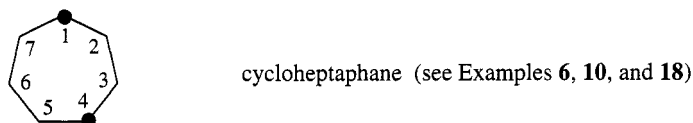
In the simplified skeletal name 'nonaphane', the numerical term 'nona' indicates that there are nine nodes in the simplified parent skeleton and the term 'phane' indicates the presence of at least one node representing a multiatomic (cyclic) structural unit. The locant set '1,3,6,9' is lower than '1,4,7,9', and is therefore correct.

#### PhI-2.1.2. Monocyclic simplified skeletons

The name of a monocyclic simplified parent skeleton consists of the prefix 'cyclo', followed by the name of the corresponding unbranched acyclic simplified parent skeleton (see PhI-2.1.1). The nodes of the cyclic graph are numbered consecutively and 'superatoms' are given preference for low numbers.

*Note:* The name 'cyclopropaphane' rather than 'cyclotriphane' has been used in the *Beilstein Handbook of Organic Chemistry* (ref. 14), but neither 'cyclopropaphane' nor 'cyclobutaphane' is used in these recommendations.

Example:



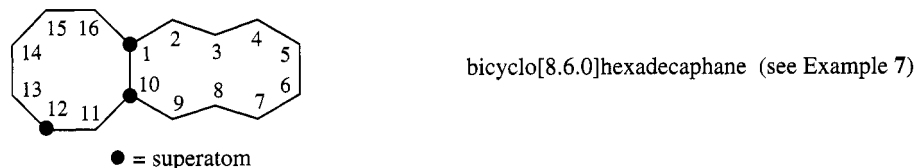
● = superatom

In the simplified skeletal name 'cycloheptaphane', the numerical term 'hepta' indicates that there are seven nodes in the simplified parent skeleton. The term 'phane' indicates the presence of at least one node representing a multiatomic (cyclic) structural unit, and the prefix 'cyclo' indicates that the graph is monocyclic. The locant '1' must be assigned to a 'superatom'; the locant set '1,4' is lower than '1,5' and is therefore correct.

#### PhI-2.1.3. Multicyclic simplified skeletons without free spiro nodes

The name of a simplified skeleton that contains bridgehead nodes (refs 1c,2c), but no free spiro nodes (refs 1d,2d) is formed in accordance with principles of the extended von Baeyer system (refs 1e,2e,15). Superatoms are given preference for low numbers.

Example:



In the simplified skeletal name 'bicyclo[8.6.0]hexadecaphane', the prefix 'bicyclo' indicates that there are two rings. The bridge descriptor describes the ring structure in terms of a sixteen-membered main ring [8 + 6 + 2 (the bridgehead nodes)] with a bridge consisting of a bond, i.e., zero nodes, which divides the main ring into an eight-membered and a ten-membered ring. The numerical term 'hexadeca' denotes the presence of sixteen skeletal nodes and the term 'phane' indicates that at least one node represents a multiatomic (cyclic) structural unit. The locant set '1,10,12' is lower than '1,10,15', and is therefore correct.



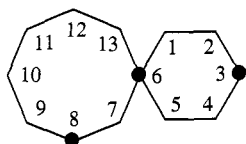
*PhI-2.1.4. Multicyclic simplified skeletons with spiro nodes but no bridgehead nodes*

The name of a multicyclic simplified skeleton with 'free spiro unions' (refs 1d,2d) but no bridgehead nodes (refs 1c,2c) is formed according to the normal rules for naming spiro hydrocarbons having only monocyclic components (refs 1f,1g,2f,2g,16).

*PhI-2.1.4.1. Monospiro simplified skeletons*

The name of a simplified skeleton having a single free spiro node linking two monocyclic simplified skeletons is formed according to the normal rules for naming monospiro hydrocarbons having only two monocyclic components (refs 1f,2f,16). Superatoms are given preference for low numbers.

Example:



spiro[5.7]tridecaphane (see Example 15)

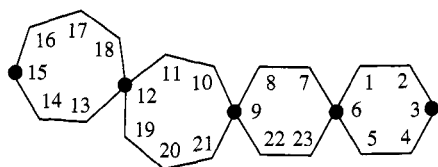
● = superatom

In the simplified skeletal name 'spiro[5.7]tridecaphane', the term 'spiro' indicates that there is one free spiro union. The ring descriptor describes the ring structure in terms of a six-membered ring [5 + 1 (the spiro node)] and an eight-membered ring [7 + 1 (the spiro node)]. The numerical term 'trideca' denotes the presence of thirteen skeletal nodes and the term 'phane' indicates that at least one node represents a multiatomic (cyclic) structural unit. The locant set '3,6,8' is lower than '3,6,12', and is therefore correct.

*PhI-2.1.4.2. Linear unbranched multispiro simplified skeletons*

The name of a simplified skeleton consisting of an unbranched linear arrangement of monocyclic simplified skeletons each connected by a free spiro union is formed according to the normal rules for naming dispiro and polyspiro hydrocarbons having only monocyclic components (refs 1g,2g,16). Superatoms are given preference for low numbers. Branched multispiro simplified skeletons are possible beginning with trispiro systems. In reference 16, the use of spiro atom locants as superscripts is recommended for all spiro systems consisting of only monocyclic components beginning with trispiro. These locants distinguish between unbranched and branched systems.

Example:



trispiro[5.2.2.6<sup>12</sup>.3<sup>9</sup>.2<sup>6</sup>]tricosaphane (see Example 17)

● = superatom

In the simplified skeletal name 'trispiro[5.2.2.6<sup>12</sup>.3<sup>9</sup>.2<sup>6</sup>]tricosaphane', the term 'spiro' preceded by the numerical term 'tri' indicates the presence of three free spiro unions. The ring descriptor describes the ring structure in terms of, in order, a terminal six-membered ring [5 + 1 (the spiro atom)], another six-membered ring [2 + 2 (the second and sixth numbers) + 2 (the spiro atoms)], a seven-membered ring [2 + 3 (the third and fifth numbers) + 2 (the spiro atoms)], and a seven-membered terminal ring [6 + 1 (the spiro atom)]. The superscript locants indicate that the fourth, fifth, and sixth segments between the spiro atoms terminate at the spiro atoms with the locants 12, 9, and 6, respectively. The numerical term 'tricosaphane' denotes the presence of twenty-three skeletal nodes and the term 'phane' indicates that at least one node represents a multiatomic (cyclic) structural unit. The locant set '3,6,9,12,15' is lower than '3,6,9,12,16' and is therefore correct.

## PhI-2.2. Amplification prefixes

An amplification prefix specifies a multiatomic (cyclic) unit of structure that replaces a node of a simplified skeleton, thereby identifying a 'superatom'. Amplification prefixes are immediately followed by the simplified skeletal name forming an inseparable unit, the phane parent name. In the terminology of published IUPAC rules and recommendations for naming organic compounds, such prefixes are called 'nondetachable' (refs 1h,2h). Phane nomenclature requires a separate amplification prefix for each ring or ring system in the structure.

### PhI-2.2.1. Parent hydride names for deriving amplification prefix names

*PhI-2.2.1.1.* An amplification prefix name is derived from a name for a cyclic parent hydride. The latter includes monocycles and polycycles with the maximum number of noncumulative double bonds ['mancude' (ref. 17) systems] (refs 1i,2i,18), bridged fused ring systems (refs 1j,2j,18), saturated monocycles (refs 1k,2k,19), saturated bicycloalkanes and polycycloalkanes (von Baeyer ring systems) (refs 1e,2e,15), and spiroalkanes (refs 1f,1g,2f,2g,16). Numbering of the cyclic parent hydride from which the amplification prefix is derived is retained.

*Note:* Ring systems with names that include fusion prefixes, such as 'benzo' in 'benzo[a]-acridine', and bridge prefixes, such as 'ethano' in '9,10-ethanoanthracene' are approved names for deriving amplification prefix names. Thus, fusion and bridging prefixes are not used with phane parent hydride names.

*PhI-2.2.1.2.* Names with 'hydro' prefixes, such as '9,10-dihydroanthracene', or subtractive endings, such as 'ene' in 'cyclohexene', are not used to derive names for amplification prefixes. 'Spirobi-' names, such as '1,1'-spirobi[indene]', spiro ring systems with at least one fused or polycycloalkane component, such as 'spiro[1,3-dioxolane-2,1'-indene]', ring assembly names, such as '2,2'-binaphthalene', and ring names containing traditional skeletal replacement ('a') prefixes, such as 'oxa', 'aza', 'sila' in names like 1-azabicyclo[2.2.2]octane and 5-silaspiro[4.5]decane are also not approved for forming amplification prefix names.

*PhI-2.2.1.3.* The term 'parent hydride name' excludes names with substitutive suffixes, such as 'ol', 'one', 'oic (acid)', and 'ylum', from use for deriving amplification prefix names. Similarly, names with substitutive prefixes, such as 'ethyl' or 'dibromo', are excluded, as are functional class names and conjunctive names, such as 'benzyl chloride' and 'benzeneacetic acid', respectively.

*PhI-2.2.1.4.* Names corresponding to substituted rings or ring systems, such as 'toluene' and 'styrene', or functional parent compounds, such as 'anisole' and 'aniline', are not acceptable for derivation of amplification prefix names. However, names of stereoparent hydrides, such as 'gonane' and 'morphinane', are acceptable.

*PhI-2.2.1.5.* Names corresponding to partially hydrogenated fused ring systems, such as 'indane' and 'chromane', are not acceptable for derivation of amplification prefix names. Modifications of the state of hydrogenation are made to the complete phane name and not to individual component names; this methodology will be described in a subsequent set of recommendations.

### PhI-2.2.2. Formation of amplification prefix names

The name of an amplification prefix is formed by adding the letter 'a' to the name of the corresponding parent hydride, with elision of the final letter 'e', if present, for example, 'benzena', 'furana', 'pyridina', 'piperidina', 'pyrrola', 'pyrrolidina', and '1-benzothiophena'.

*PhI-2.2.3. Order of citation of amplification prefixes*

The order of citation of two or more amplification prefixes in a phane parent name is determined by the order of seniority of rings and ring systems. Six criteria, with illustrative examples, are listed here. A full comprehensive order is under review by the Commission.

- All heterocycles are senior to carbocycles:  
pyridine > phenanthrene
- A heterocycle with a heteroatom as early as possible in the following list is preferred:  
N > O > S > Se > Te > P > As > Sb > Bi > Si > Ge > Sn > Pb > B  
pyrrolidine > furan > thiophene
- A ring system with the greater number of rings is preferred:  
quinoline > pyridine  
phenanthrene > naphthalene > benzene
- A ring or ring system with the greater number of atoms in the largest individual ring at the first point of difference is preferred:  
naphthalene > indene  
pyridine > 1,2-oxazole
- A ring or ring system with the greater number of heteroatoms of any kind is preferred:  
pyrimidine > pyridine  
1,2,5-oxadiazole > pyrrole
- A ring or ring system in the lower state of hydrogenation is preferred:  
pyridine > piperidine  
benzene > cyclohexane

*PhI-2.2.4. Multiple identical amplifiants*

Amplifiants occurring more than once in a phane parent skeleton are described by an appropriate multiplicative term, either 'di', 'tri', etc., or 'bis', 'tris', etc., prefixed to the name of the amplifiant. It is not necessary that the identical amplifiants also have identical attachment locants.

*PhI-2.2.4.1.* The multiplicative terms 'di', 'tri', etc., are used in front of simple amplification prefix names.

Examples:

pyrimidinatripyridinanonaphane (see Example 1)  
(not pyrimidinapyridinapyridinapyridinanonaphane)

dibenzenacycloheptaphane (see Example 10)  
(not benzenabenzenacycloheptaphane)

*PhI-2.2.4.2.* The multiplicative terms 'bis', 'tris', etc., are used before an amplification prefix when it begins with a multiplicative term, as in 'bicyclo[2.2.2]octane', '1,3-dioxole', and '4,7-dinorgonane' or it begins with a name component that could be preceded by a multiplicative prefix indicating a multiple occurrence of that name component, as in '1,4-oxazine', '2-benzoxepine', and '1,4-methanonaphthalene'.

**PhI-2.3. Superatom locants and amplifiant attachment locants**

After the simplified skeletal name and the amplification prefix names have been determined, the phane parent hydride name is completed by adding the locants for the superatoms (see PhI-1.3) and the attachment locants (see PhI-1.5). These locants are cited before an amplification prefix; the superatom

locant is cited first followed by the attachment locants enclosed in parentheses. Specific locants are determined from the numbering procedures given in PhI-3.

In the phane parent hydride name 3(5,2)-pyridina-1(3,1)-piperidina-6(3,1)-naphthalenacyclononaphane (see Example 2), the locants '3', '1' and '6' are superatom locants and the locants in parentheses, '(5,2)', '(3,1)' and '(3,1)', are the respective attachment locants for the three amplificants.

#### *PhI-2.3.1. Superatom locants*

Superatom locants specify the nodes of the simplified skeleton that are replaced by the amplificants specified by the amplification prefixes. Superatom locants are assigned the lowest locants (refs 1b,2b) of the phane parent skeleton consistent with the numbering of the class to which it belongs (see PhI-2.1.1 through PhI-2.1.4). An amplification prefix preceded by a multiplicative term indicating the presence of like amplificants requires the appropriate number of superatom locants, which are cited in ascending numerical order.

In the phane parent hydride name 1(1,3),4(1,4)-dibenzenacycloheptaphane (see Example 10), the numerical prefix 'di' requires the two superatom locants '1' and '4' which appear in the order '1,4', each in front of the appropriate parenthetical attachment locants (see PhI-2.3.2).

When like amplificants also have identical attachment locants as described in PhI-2.3.2.1, below, their attachment locants are arranged in ascending numerical order of the first cited corresponding superatom locant.

In the phane parent hydride name 1,9(1),3,5,7(1,4)-pentabenzanonaphane (see the name in step 1, Example 21), the identical attachment locant sets '(1,4)' for three of the five benzene amplificants are cited only once and follow the superatom locant set '3,5,7'; the two terminal benzene amplificants with the same attachment locant '(1)' are cited only once and follow the superatom locant set '1,9'.

In the phane parent hydride name 3,15(1,4),6(1,4,2,5),9(1,2,5,4),12(1,5,2,4)-pentabenzatripiro[5.2.2.6<sup>12</sup>.3<sup>9</sup>.2<sup>6</sup>]tricosaphane (see Example 17), the numerical prefix 'penta' requires five superatom locants, 3,6,9,12,15. In order to show that amplificants '3' and '15' have the identical attachment locant set '(1,4)', they are placed, in ascending order, before this attachment locant set, i.e., 3,15(1,4). See also Example 1.

#### *PhI-2.3.2. Attachment locants*

The locants enclosed in parentheses in a phane parent hydride name are the attachment locants of the ampicant whose position in the phane parent skeleton is specified by a preceding superatom locant. The specific order of the attachment locants in the set describes precisely how their respective ampicant is attached to the rest of the phane parent skeleton. Amplicants retain the locants of the cyclic parent hydride from which they are derived (see PhI-2.2.1.1).

*PhI-2.3.2.1.* Identical attachment locant sets for multiple identical amplificants are cited only once in a name; they follow the set of superatom locants corresponding to the identical amplificants.

In the phane parent hydride name 4(5,2),12(3,5)-dipyridina-1,8(1,3,5)-dibenzenabicyclo[6.6.0]tetradecaphane (see Example 11), the identical locant sets for the two benzene amplificants '(1,3,5)' are cited only once and follow the superatom locant set '1,8'; the nonidentical attachment locant sets '(5,2)' and '(3,5)' for the two pyridine amplificants must be cited separately.

*PhI-2.3.2.2.* The locants in an attachment locant set are arranged so that of any two locants the one cited first is adjacent to the lower locant of the phane parent skeleton.

In the phane parent hydride name 1(4)-pyrimidina-3,6(5,2),9(3)-tripyridinanonaphane (see Example 1), the arrangement of the locants in the attachment locant set '(5,2)' for superatoms '3' and '6'

indicate that the attachment locant '5' is adjacent to locants '2' and '5' of the phane parent skeleton, respectively.

*Note:* If the adjacent node of a phane parent skeleton is a superatom, the real adjacent atom is another attachment atom, which has its own superatom locant and attachment locant set. This superatom locant is considered first (the corresponding attachment locant is important in particular cases, which will be discussed in a later set of recommendations).

### PHI-3. NUMBERING OF PHANE PARENT HYDRIDES

The following rules are used for numbering phane parent hydrides. These rules are hierarchical, i.e., each particular rule is applied only to alternatives not eliminated by preceding rules.

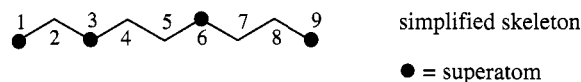
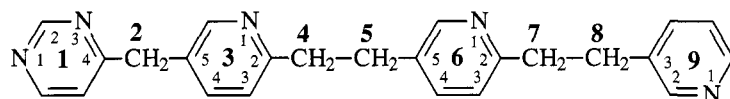
#### Phi-3.1. Numbering of phane parent skeletons and amplificants

*Phi-3.1.1.* The numbering of a phane parent skeleton is first determined by the rules governing the appropriate skeletal class to which it belongs (see Phi-2.1). When, because of skeletal symmetry, these rules leave alternatives, the numbering that gives the lowest set of locants for the superatoms is preferred. The lowest set of locants (refs 1b,2b) 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.

*Phi-3.1.2.* Numbering of an amplificant is determined primarily by the numbering rules that apply to the parent hydride from which the amplificant is derived. When there is a choice, the established procedure for lowest locants is applied. The lowest locant set (refs 1b,2b) 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.

These two rules are exemplified by the following examples.

Example 1.



1(4)-pyrimidina-3,6(5,2),9(3)-tripyridinanonaphane

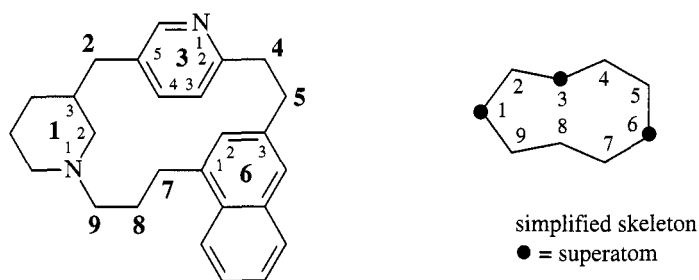
*not* 9(4)-pyrimidina-1(3),4,7(2,5)-tripyridinanonaphane (See Phi-2.1.1 and Phi-3.1.1; the superatom locant set of the correct name, '1,3,6,9', is lower than '1,4,7,9'.)

*not* 1(4)-pyrimidina-3,6(2,5),9(3)-tripyridinanonaphane [See Phi-2.3.2.2; the first locant of the attachment locant set '(2,5)' is not the locant adjacent to the lower locant of the simplified skeleton.]

*not* 1(4)-pyrimidina-3(5,2),6(5,2),9(3)-tripyridinanonaphane [See Phi-2.3.2.1; the identical attachment locant sets '(5,2)' must be contracted to '3,6(5,2)'.]

*not* 1(4)-pyrimidina-3,6(3,6),9(3)-tripyridinanonaphane [See Phi-3.1.2; the attachment locant set '(5,2)' of the pyridine amplificant in the correct name, written in the ascending numerical order '(2,5)' for comparison, is lower than the set '(3,6)'.]

## Example 2.

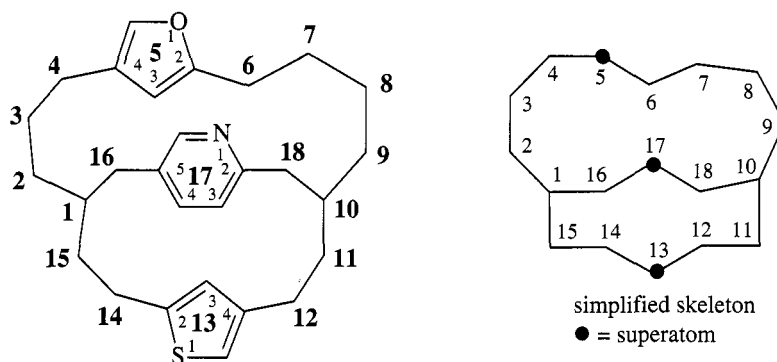


3(5,2)-pyridina-1(3,1)-piperidina-6(3,1)-naphthalenacyclononaphane

not 7(5,2)-pyridina-5(1,3)-piperidina-1(1,3)-naphthalenacyclononaphane (See PhI-2.1.2 and PhI-3.1.1; the superatom locant set of the correct name, '1,3,6', is lower than the locant set '1,5,7'.)

not 3(2,5)-pyridina-1(1,3)-piperidina-6(1,3)-naphthalenacyclononaphane [See PhI-2.3.2.2; the first locant of each of the attachment locant sets '(2,5)', '(1,3)', and '(1,3)' for the pyridine, piperidine, and naphthalene amplificants, respectively, is not the locant adjacent to the lower locant of the phane parent skeleton.]

## Example 3.



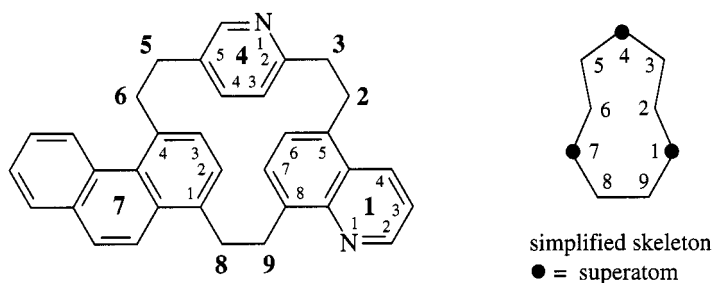
17(5,2)-pyridina-5(4,2)-furana-13(4,2)-thiophenabicyclo[8.5.3]octadecaphane

not 17(2,5)-pyridina-11(4,2)-furana-4(4,2)-thiophenabicyclo[8.5.3]octadecaphane

not 3(5,2)-pyridina-14(4,2)-furana-8(4,2)-thiophenabicyclo[8.5.3]octadecaphane (See PhI-2.1.3; the superatom locants in the incorrect names, '4,11,17' and '3,8,14', are not allowed by the numbering rules for the bicyclic system.)

*PhI-3.1.3.* Amplification of symmetrical simplified phane skeletons with at least two superatoms representing different amplificants results in the loss of symmetry and creates numbering alternatives. In such cases, the lower available superatom locant is assigned to an amplificant that appears earlier in the seniority of rings and ring systems (see PhI-2.2.3). The application of this procedure may require a sequence of steps. First, the lowest available superatom locant(s) is (are) assigned to the amplificants appearing first in the seniority order. Then, the same procedure is applied successively to assign remaining superatom locants to the rest of the amplificants.

## Example 4.

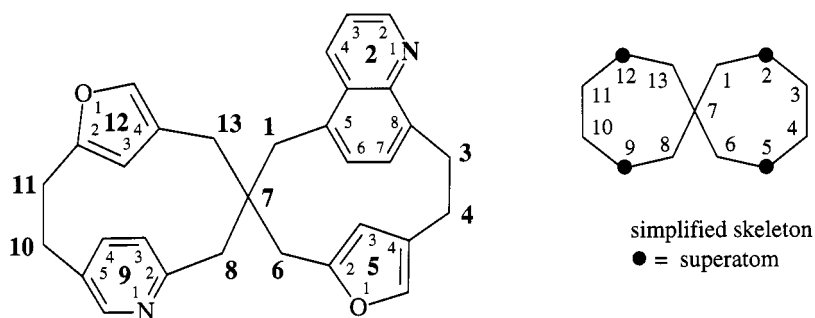


1(5,8)-quinolina-4(2,5)-pyridina-7(4,1)-phenanthrenacyclononaphane

*not* 1(8,5)-quinolina-7(5,2)-pyridina-4(1,4)-phenanthrenacyclononaphane [The senior amplificant is quinoline (see PhI-2.2.3) and must receive the lowest superatom locant, '1'; the pyridine amplificant is second in seniority (see PhI- 2.2.3) and therefore must be given the second lowest superatom locant, '4'.]

*not* 1(5,8)-quinolina-4(2,5)-pyridina-7(1,4)-phenanthrenacyclononaphane [See PhI-2.3.2.2; the attachment locants of the phenanthrene amplificant, '(1,4)' are not correctly cited; the first locant of the attachment locant set is not the locant adjacent to the lower locant of the phane parent skeleton, '6'.]

## Example 5.

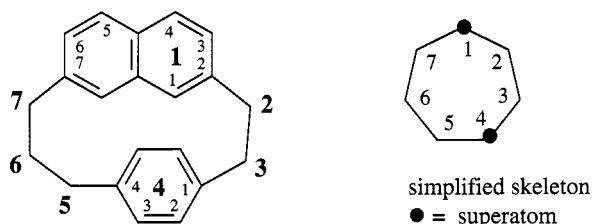


2(5,8)-quinolina-9(2,5)-pyridina-5(4,2),12(2,4)-difuranaspiro[6.6]tridecaphane

*not* 2(5,8)-quinolina-12(5,2)-pyridina-5,9(4,2)-difuranaspiro[6.6]tridecaphane [The senior amplificant is quinoline (see PhI-2.2.3) and must be given the lowest superatom locant, '2'; the pyridine amplificant is second in seniority (see PhI-2.2.3) and must be assigned the next available lowest superatom locant, '9'; therefore the furan amplificants have the superatom locants '5' and '12'.]

*PhI-3.1.4.* When, because of symmetry, PhI-3.1.2 leaves a choice, an amplificant is numbered in such a way that the lower attachment locant is adjacent to the lower locant of the phane parent skeleton (see also PhI-2.3.2.2).

## Example 6.



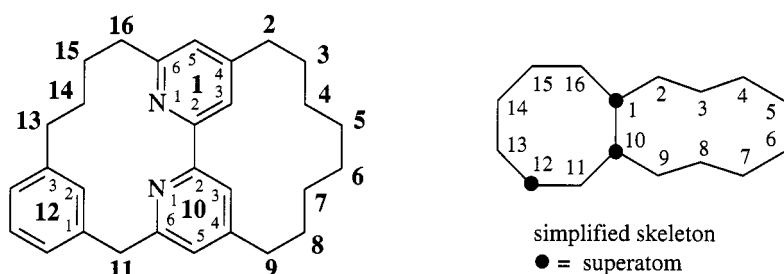
1(2,7)-naphthalena-4(1,4)-benzenacycloheptaphane

[See PhI-2.1.2 and PhI-3.1.1; the lowest locant set for the superatoms in the phane parent skeleton is '1,4'; the senior amplificant, naphthalene (see PhI-2.2.3), must be assigned the superatom locant '1'.]

not 1(2,7)-naphthalena-4(4,1)-benzenacycloheptaphane

not 1(7,2)-naphthalena-4(4,1)-benzenacycloheptaphane (The correct citation for the attachment locant sets, '1,4' for benzene and '2,7' for naphthalene, places the lower attachment locant adjacent to the lower locant of the phane skeleton.)

Example 7.



1(4,2,6),10(2,4,6)-dipyridina-12(1,3)-benzenabicyclo[8.6.0]hexadecaphane [The attachment locant sets of both pyridine amplificants are '(2,4,6)'. However, the attachment locant sets of each amplificant must follow PhI-2.3.2.2, i.e., the lower locant of each attachment locant set must be next to the lowest possible locant of the phane skeleton. The attachment locant '4' in each pyridine amplificant is invariant. Locant '2' of amplificant '1' must be adjacent to phane skeletal locant '10' (not '16') and locant '2' of amplificant '10' must be adjacent to phane skeletal locant '1' (not '11').]

not 1(4,2,6),10(2,4,6)-dipyridina-15(1,3)-benzenabicyclo[8.6.0]hexadecaphane (See PhI-2.1.3 and PhI-3.1.1; the superatom locant set in the correct name, '1,10,12', is lower than '1,10,15'.)

not 1,10(2,4,6)-dipyridina-12(1,3)-benzenabicyclo[8.6.0]hexadecaphane (See PhI-2.3.2.1; since the attachment locant sets of the two pyridine amplificants are not identical, they must be cited separately.)

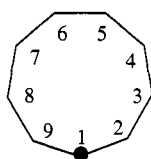
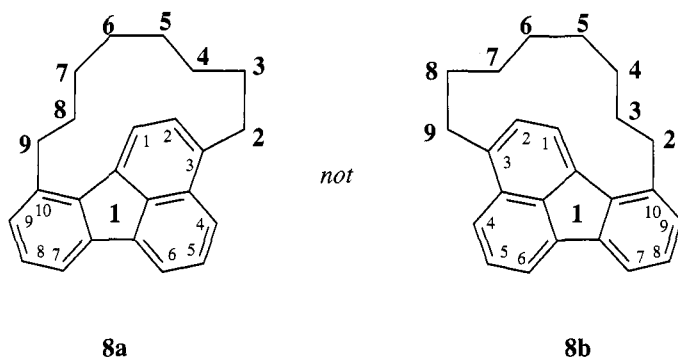
### PhI-3.2. Numbering of simplified phane skeletons with respect to amplificant numbering

Numbering alternatives occur in symmetrical simplified parent skeletons when a single amplificant is unsymmetrical or when two or more amplificants are identical but have different attachment locants. Choice among such alternatives is made according to the following rules.

*PhI-3.2.1.* When a single amplificant is unsymmetrical, the lower locant of the phane parent skeleton must be adjacent to the lower attachment locant of the amplificant.



## Example 8.



simplified skeleton  
● = superatom

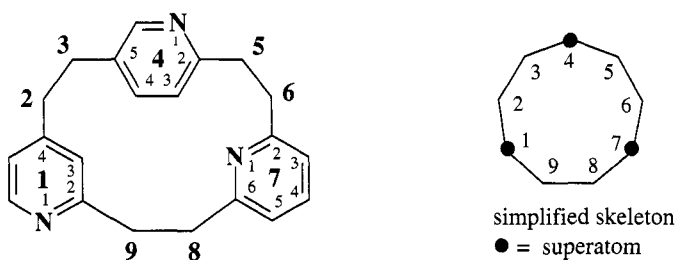
1(3,10)-fluoranthenacyclononaphane (8a)

not 1(10,3)-fluoranthenacyclononaphane (8b) (The lower attachment locant '3' must be adjacent to the lower locant of the phane skeletal locant '2'.)

not 1(4,7)-fluoranthenacyclononaphane [See PhI-3.1.2; the attachment locant set in the correct name, '(3,10)', is lower than '(4,7)'.]

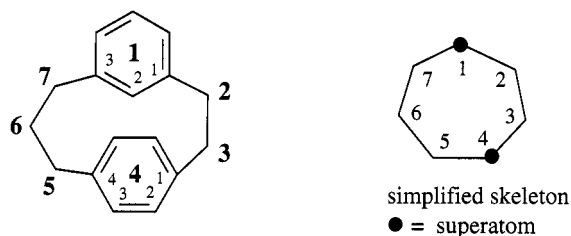
*PhI-3.2.2.* When two amplificants can be given the lower of two superatom locants, the lower locant is assigned to the superatom representing the amplificant with the lower set of attachment locants. When necessary, this procedure is applied to other amplificants in accordance with their order of seniority until two or more identical amplificants have different attachment locants (see Example 12).

## Example 9.



1(4,2),4(5,2),7(2,6)-tripyridinacyclononaphane [The attachment locant sets '(2,4)', '(2,5)', and '(2,6)' must be assigned to superatoms '1', '4', and '7' respectively. The arrangement of the locants in each set is governed by PhI-2.3.2.2.]

## Example 10.

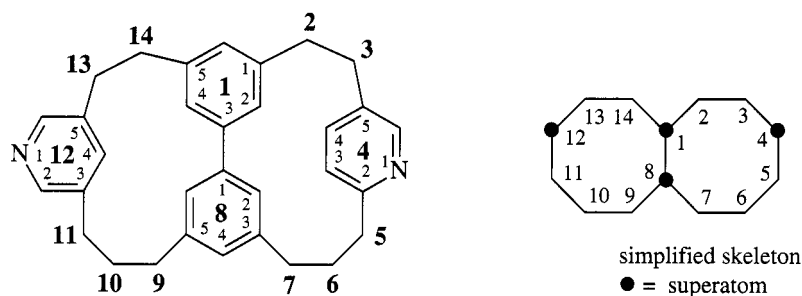


1(1,3),4(1,4)-dibenzencycloheptaphane

*not* 1(1,4),4(1,3)-dibenzencycloheptaphane [The lower attachment locant set '(1,3)' is not associated with the superatom having the lower locant.]

*not* 1(1,3),4(4,1)-dibenzencycloheptaphane [See PhI-2.3.2.2 and PhI-3.1.4; in the attachment locant set '(4,1)', the first locant is not the one adjacent to the lower locant of the phane parent skeleton.]

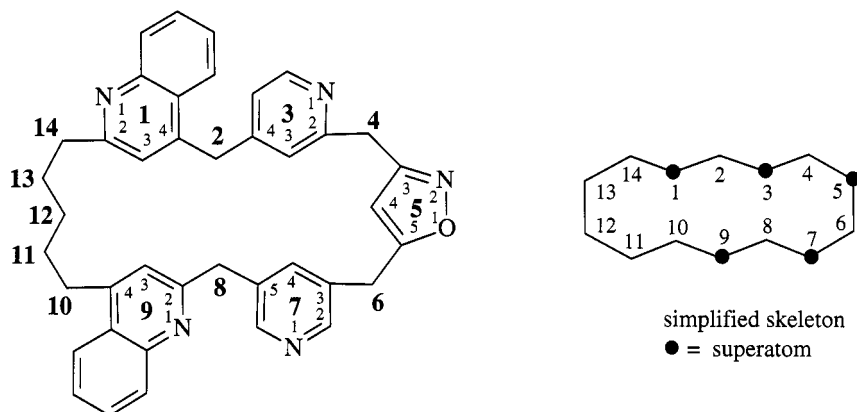
## Example 11.



4(5,2),12(3,5)-dipyridina-1,8(1,3,5)-dibenzencyclo[6.6.0]tetradecaphane

*not* 4(3,5),12(2,5)-dipyridina-1,8(1,3,5)-dibenzencyclo[6.6.0]tetradecaphane [For the pyridine amplificants, the attachment locant set '(5,2)', when compared in ascending numerical order, i.e., '(2,5)', is lower than '(3,5)'; therefore the pyridine amplificant with the locant set '(5,2)' must be associated with the lower superatom locant '4'.]

## Example 12.



Example 12. (cont'd.)

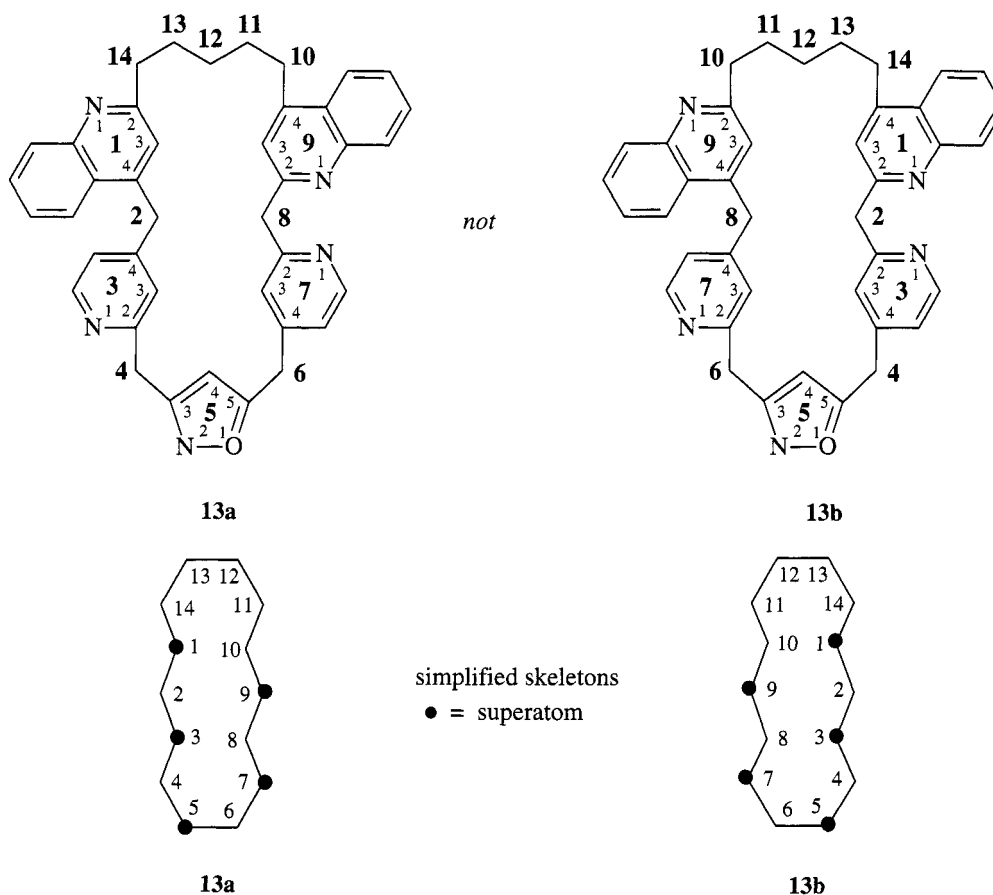
1(4,2),9(2,4)-diquinolina-3(4,2),7(3,5)-dipyridina-5(3,5)-1,2-oxazolacyclotetradecaphane

not 1(2,4),9(4,2)-diquinolina-3(5,3),7(2,4)-dipyridina-5(5,3)-1,2-oxazolacyclotetradecaphane

[The attachment locant sets for the senior quinoline amplificants (see PhI-2.2.3), '(4,2)' and '(2,4)', respectively, when compared in ascending numerical order are the same, but when the attachment locant sets for the pyridine amplificants, '(4,2)' and '(5,3)', respectively, are compared in ascending numerical order, i.e., '(2,4)' with '(3,5)', the former is lower and therefore the attachment locant set '(4,2)' is associated with the superatom with the lower locant '3'.]

PhI-3.2.3. If, after the application of PhI-3.2.2, a choice is still necessary and a single unsymmetrical amplificant remains, PhI-3.2.1 is applied to the single unsymmetrical amplificant.

Example 13.

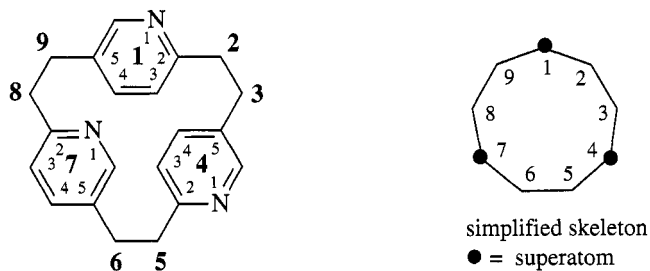


1(4,2),9(2,4)-diquinolina-3,7(4,2)-dipyridina-5(3,5)-1,2-oxazolacyclotetradecaphane (13a)

not 1(2,4),9(4,2)-diquinolina-3,7(2,4)-dipyridina-5(5,3)-1,2-oxazolacyclotetradecaphane (13b) [Each of the identical pairs of amplificants, quinoline and pyridine, have identical attachment locants, '(2,4)' and '(2,4)', respectively. The single unsymmetrical amplificant, 1,2-oxazole, remains to which PhI-3.2.1 applies; its lower attachment locant '3' must be adjacent to the lower locant of the parent phane skeleton, '4'.]

Ph-I-3.2.4. When two numberings for a simplified phane skeleton are still possible, the preferred numbering is that which gives the lower locant set when attachment locants of all amplificants, as they appear in the name, are compared in the increasing order of their corresponding superatom locants.

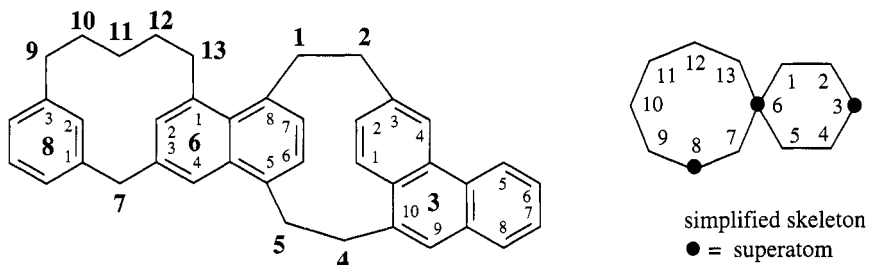
## Example 14.



1(2,5),4,7(5,2)-tripyridinacyclononaphane

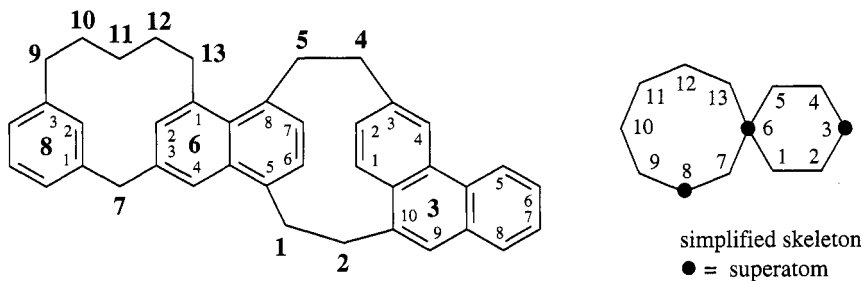
not 1(5,2),4,7(2,5)-tripyridinacyclononaphane [When compared in the order of increasing value of the corresponding superatoms, the set of amplificant locants '(2,5)(5,2)(5,2)' in the correct name is lower than '(5,2)(2,5)(2,5)'.]

## Example 15.



15a

not



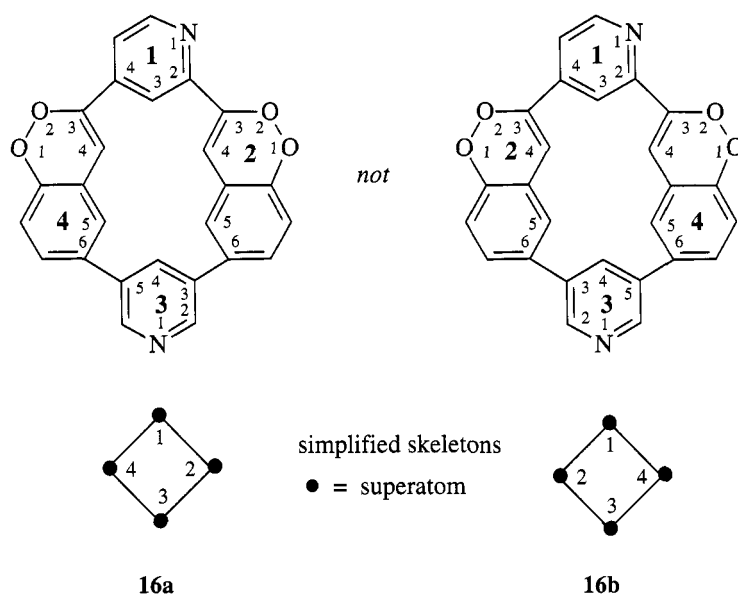
15b

3(3,10)-phenanthrena-6(8,5,3,1)-naphthalena-8(1,3)-benzenaspiro[5.7]tridecaphane (15a)

not 3(10,3)-phenanthrena-6(5,8,3,1)-naphthalena-8(1,3)-benzenaspiro[5.7]tridecaphane (15b)

[The set of attachment locants '(3,10)(8,5,3,1)(1,3)' in the name for 15a cited for comparison in order of the increasing value of their corresponding superatom locants, is lower than '(10,3)(5,8,3,1)(1,3)', the corresponding set of attachment locants in the name for 15b.]

## Example 16.

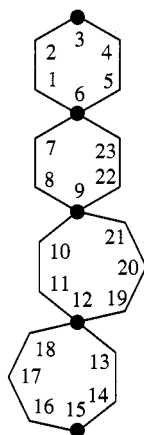
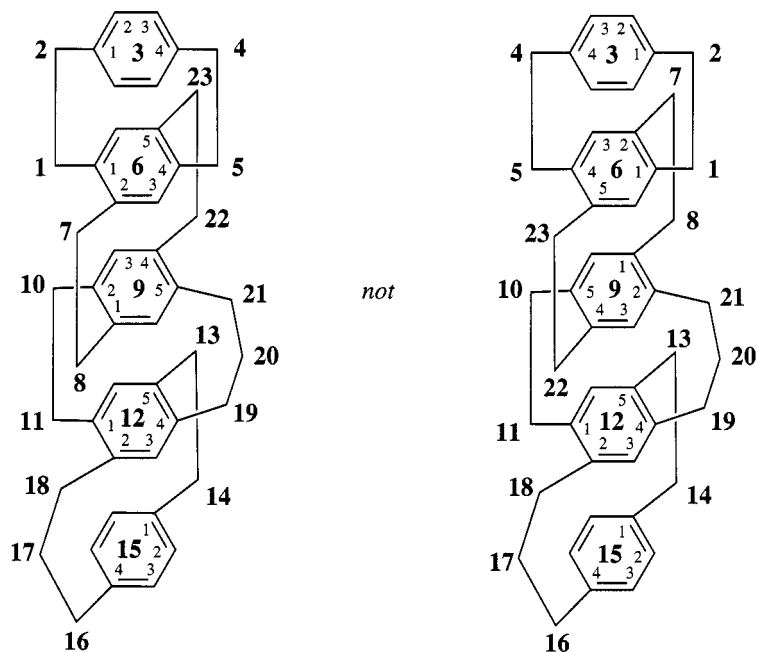


1(2,4),3(3,5)-dipyridina-2,4(3,6)-bis(1,2-benzodioxina)cyclotetraphane (16a)

not 1(4,2),3(3,5)-dipyridina-2,4(3,6)-bis(1,2-benzodioxina)cyclotetraphane (16b) [When compared in the order of the increasing value of the corresponding superatoms, the set of attachment locants in 16a, '(2,4)(3,6)(3,5)(3,6)', is lower than the set '(4,2)(3,6)(3,5)(3,6)' in 16b.]

*Note:* A guide to construction of the name for Example 16. According to PhI-3.2.2, the pyridine amplificant with the attachment locants '(2,4)' must be given the superatom locant '1'. Amplificant '4' is adjacent to amplifiants '1' and '3'. This is important for the citation of amplificant locants, which, are '(3,6)' and not '(6,3)', because according to PhI-2.3.2.2, the amplificant locant adjacent to the lower skeletal locant must be cited first.

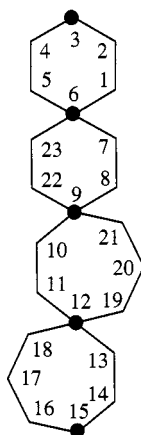
## Example 17.



17a

simplified skeletons

● = superatom



17b

3,15(1,4),6(1,4,2,5),9(1,2,5,4),12(1,5,2,4)-pentabenzetrisspiro[5.2.2.6<sup>12</sup>.3<sup>9</sup>.2<sup>6</sup>]tricosaphane (17a)

not 3,15(1,4),6(1,4,2,5),9,12(1,5,2,4)-pentabenzetrisspiro[5.2.2.6<sup>12</sup>.3<sup>9</sup>.2<sup>6</sup>]tricosaphane (17b)

[The set of attachment locants '(1,4)(1,4,2,5)(1,2,5,4)(1,5,2,4)(1,4)' in the name for 17a, cited for comparison in order of the increasing value of their corresponding superatom locants, is lower than the corresponding set of attachment locants in the name for 17b,

'(1,4)(1,4,2,5)(1,5,2,4)(1,5,2,4)(1,4)'.]

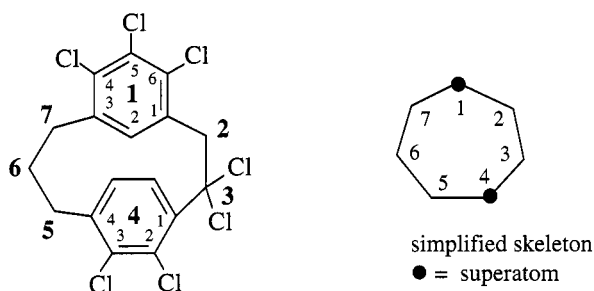
### Phi-3.3. Numbering of phane parent hydrides

*Phi-3.3.1.* In a phane parent hydride name, the locants for atoms that do not belong to amplificants are the locants of the simplified phane skeleton. However, locants for the atoms of the amplificants must be distinguished from the arabic number locants of the simplified skeleton. Thus, locants for amplificant atoms are constructed by citing the actual locants of the amplificant as superscripts to the locant of the superatom that represents the amplificant in the simplified skeleton.

*PhI-3.3.2.* In a substituted phane parent hydride name, a series of composite locants based on the same superatom locant must not be contracted. As it is the rule for citing locants in front of detachable prefixes, there must be a number of locants corresponding to the multiplicative prefix, 'di', 'tri', etc., in front of the prefix.

*PhI-3.3.3.* The seniority of a composite locant is determined first on the basis of its primary locants, i.e., the locants of the phane parent skeleton, and, if these locants are identical, on the basis of the complete composite locant itself, i.e., the primary locant and its superscripts.

Example 18.

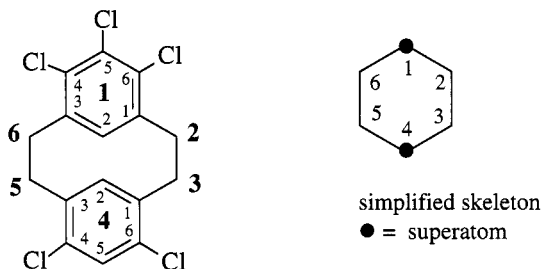


$1^4, 1^5, 1^6, 3, 3, 4^2, 4^3$ -heptachloro-1(1,3),4(1,4)-dibenzenacycloheptaphane

not  $1^{4,5,6}, 3, 3, 4^{2,3}$ -heptachloro-1(1,3),4(1,4)-dibenzenacycloheptaphane (See PhI-3.3.2; superscript locants denoting positions on amplifcants are not contracted.)

not  $1^2, 1^3, 2, 2, 4^4, 4^5, 4^6$ -heptachloro-1(1,4),4(1,3)-dibenzenacycloheptaphane (See PhI-3.2.2; the amplifcant with the lower locant set is not assigned to the superatom with the lower locant.)

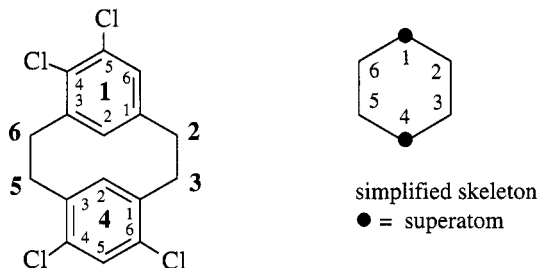
Example 19.



$1^4, 1^5, 1^6, 4^4, 4^6$ -pentachloro-1,4(1,3)-dibenzenacyclohexaphane

not  $1^4, 1^6, 4^4, 4^5, 4^6$ -pentachloro-1,4(1,3)-dibenzenacyclohexaphane (See PhI-3.3.3; the primary locant set 1,1,1,4,4 is lower than the locant set 1,1,4,4,4.)

Example 20.



$1^4, 1^5, 4^4, 4^6$ -tetrachloro-1,4(1,3)-dibenzenacyclohexaphane

not 1<sup>4</sup>,1<sup>6</sup>,4<sup>4</sup>,4<sup>5</sup>-tetrachloro-1,4(1,3)-dibenzenacyclohexaphane (See PhI-3.3.3; the primary locant sets, 1,1,4,4, are identical but the composite locant set 1<sup>4</sup>,1<sup>5</sup>,4<sup>4</sup>,4<sup>6</sup> is lower than 1<sup>4</sup>,1<sup>6</sup>,4<sup>4</sup>,4<sup>5</sup>.)

#### PHI-4. SKELETAL REPLACEMENT ('a') NOMENCLATURE IN PHANE NOMENCLATURE

The skeletal replacement ('a') nomenclature operation (refs 1a,2a) involves the exchange of one group of atoms, usually  $-\text{CH}_2-$  or  $>\text{CH}-$ , or an atom, usually a carbon atom, for another group or atom. It is a way of introducing heteroatoms into rings, ring systems, or chains; the heteroatoms usually belong to elements in Groups 13, 14, 15, and 16 of the Periodic Table. This replacement operation transforms an acyclic or cyclic hydrocarbon into a heteroacyclic or heterocyclic system. Skeletal replacement is always applied to parent hydrides. The result is the formation of new parent hydrides (secondary parent hydrides) from hydrocarbon parent hydrides (primary parent hydrides).

The skeletal replacement operation can be applied as well to phane parent hydrides (primary parent hydrides) to create new phane parent hydrides (secondary parent hydrides). With phane parent hydrides, skeletal replacement nomenclature is applied in two ways:

- to indicate heteroatoms in heterocyclic amplificants whose names cannot be used as amplification prefix names because they, themselves, are named by replacement nomenclature (see PhI-2.2.1.2);
- to name phane parent hydrides having heteroatoms located in the simplified parent skeleton, i.e., heteroatoms not in names of amplification prefixes.

##### PhI-4.1. Name construction

A phane parent hydride name is constructed in accordance with the principles, conventions, and rules of phane nomenclature as described in PhI-1, PhI-2, and PhI-3. All rings and ring systems of the phane parent hydride that qualify as amplificants (see PhI-2.2.1) and hydrocarbon analogs for any heterocycles that do not qualify as amplificants because skeletal replacement ('a') nomenclature must be used to form their names are analysed together in order to apply the various rules regarding priority of rings and ring systems and attachment locants described in PhI-3. A phane parent hydride name is then assembled, using allowed names for amplificants and hydrocarbon names for those amplificants whose names require the use of skeletal replacement ('a') nomenclature. Then, 'a' prefixes for amplificants that require skeletal replacement nomenclature and for heteroatoms located in the simplified parent skeleton, are introduced into the name in front of the name of the first cited amplificant.

Locants designating the 'a' prefixes are of two types depending on the location of the heteroatoms they describe. When the heteroatoms are not part of an amplificant their locants are simply those of the simplified phane parent skeleton. In the name 2,7-dithia-1(2,5)-thiophena-5(1,3)-cyclohexanacyclooctaphane (see Example 26), the locants '2' and '7' assigned to 'dithia' are those of the simplified parent skeleton. When the heteroatoms are in an amplificant whose name requires the use of skeletal replacement nomenclature, their locants are the same as those described in PhI-3.3.1 for substituents, i.e., they are composed of the locant designating the amplificant in the simplified skeleton (the superatom) and a superscript locant indicating the position of the heteroatom in the amplificant. In the name 1<sup>2</sup>,5<sup>3</sup>-dioxo-3(2,5)-furana-1,5(1,6)-dicyclododecanacycloundecaphane (see Example 29), the locants '1<sup>2</sup>' and '5<sup>3</sup>' assigned to 'dioxo' are locants denoting heteroatoms in the cyclododecane amplificants. Skeletal replacement ('a') prefixes and their locants are cited in the name in the usual order of their priority (refs 1m,2m,19a), i.e., O > S > Se > Te > N, etc., and locants for the same heteroatom are cited in ascending order of their locants, first according to the primary skeletal (superatom) locant, and then according to the increasing numerical value of the superscript numbers (see PhI-3.3.3).

##### PhI-4.2. Skeletal replacement ('a') nomenclature in simplified skeletal names

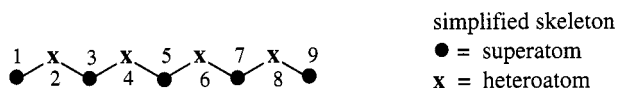
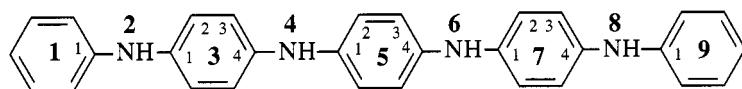
Skeletal replacement in simplified phane skeletal names is a normal skeletal replacement operation. The locants designating the position of the heteroatoms are those used to number the simplified parent skeleton. Such skeletal replacement names are constructed in two steps:



**Step 1:** The name of the phane parent hydride without heteroatoms except those in allowable amplificants (see PhI-2.2.1) is constructed;

**Step 2:** Skeletal replacement ('a') nomenclature is applied to describe heteroatoms in the phane parent hydride name formed in step 1. Locants for the heteroatoms are assigned according to the numbering of the simplified parent skeleton and cited together with the corresponding replacement ('a') prefixes in front of the name of the first cited amplificant.

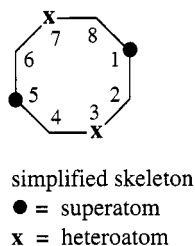
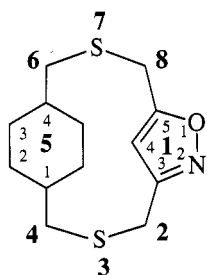
**Example 21.**



Step 1: 1,9(1),3,5,7(1,4)-pentabenzenanonaphane

Step 2: 2,4,6,8-tetraaza-1,9(1),3,5,7(1,4)-pentabenzenanonaphane

**Example 22.**



Step 1: 1(3,5)-1,2-oxazola-5(1,4)-cyclohexanacyclooctaphane

Step 2: 3,7-dithia-1(3,5)-1,2-oxazola-5(1,4)-cyclohexanacyclooctaphane

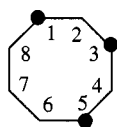
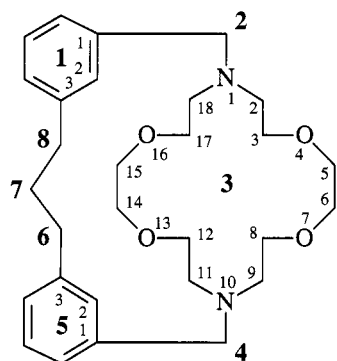
### PhI-4.3. Skeletal replacement ('a') nomenclature in amplificants

Some heterocyclic rings and ring systems can be only named by using skeletal replacement nomenclature, for example, heteromonocyclic rings having more than ten ring members (ref. 1n), heteropolycyclic compounds named by the extended von Baeyer system (refs 1o,2n,15), heterospiroalkanes (refs 1f,1g,2o,16), and hetero-polycyclic compounds whose names cannot be formed by fusion nomenclature (ref. 18). When present in a phane parent hydride as amplificants, these heterocycles must be named as hydrocarbons and the heteroatoms described by skeletal replacement nomenclature applied after construction of the phane parent hydride name. Therefore, naming of such phane parent hydrides proceeds in two steps:

**Step 1:** The name of the primary phane parent hydride is constructed based on allowed names for amplificants and hydrocarbon names for those heterocycles whose names are not allowed (PhI-2.2.1);

**Step 2:** Skeletal replacement ('a') nomenclature is applied to describe heteroatoms that are not included in the name of the phane parent hydride formed according to step 1. Locants for the heteroatoms are assigned according to the numbering of the simplified skeleton and the positions of the heteroatoms in the amplificants following the instructions in PhI-3.3 for substituents. Thus, positions of heteroatoms in amplificants are described by composite locants.

## Example 23.



simplified skeleton

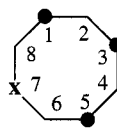
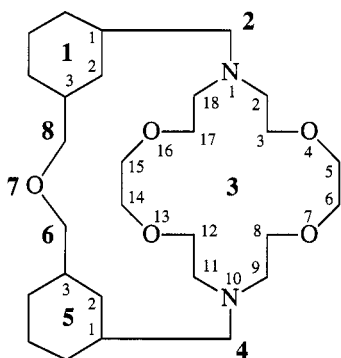
● = superatom

Step 1: 3(1,10)-cyclooctadecana-1,5(1,3)-dibenzenacyclooctaphane

Step 2: 3<sup>4,3<sup>7,3<sup>13,3<sup>16</sup></sup></sup>-tetraoxa-3<sup>1,3<sup>10</sup></sup>-diazia-3(1,10)-cyclooctadecana-1,5(1,3)-dibenzena-cyclooctaphane</sup>**PhI-4.4. Simultaneous skeletal replacement in amplificants and simplified skeletal names**

When skeletal replacement occurs in both amplificants and simplified skeletons, both PhI-4.2 and PhI-4.3 are applied.

## Example 24.



simplified skeleton

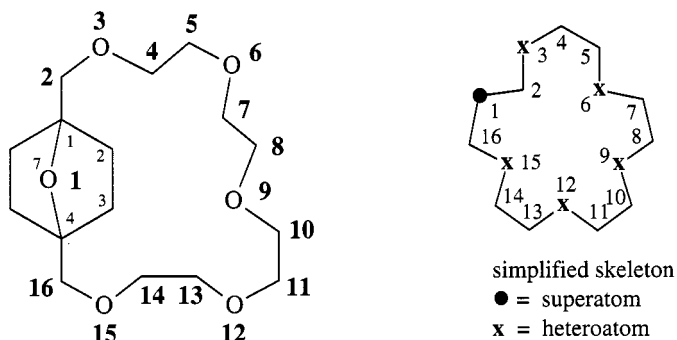
● = superatom

x = heteroatom

Step 1: 3(1,10)-cyclooctadecana-1,5(1,3)-dicyclohexanacyclooctaphane

Step 2: 3<sup>4,3<sup>7,3<sup>13,3<sup>16</sup></sup></sup>-7-pentaoxa-3<sup>1,3<sup>10</sup></sup>-diazia-3(1,10)-cyclooctadecana-1,5(1,3)-dicyclohexana-cyclooctaphane</sup>

## Example 25.



Step 1: 1(1,4)-bicyclo[2.2.1]heptanacyclohexadecaphane

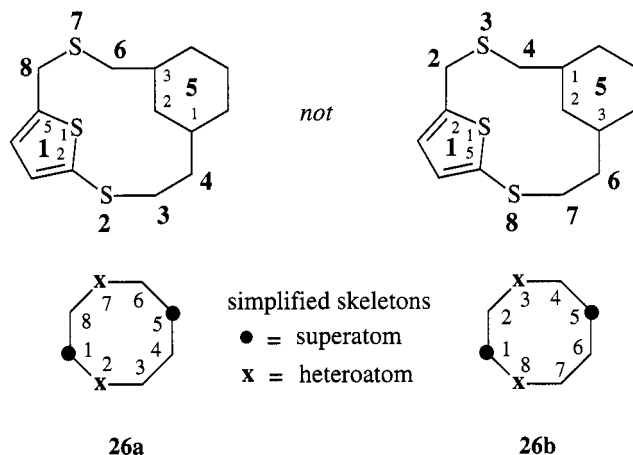
Step 2:  $1^7,3,6,9,12,15$ -hexaoxa-1(1,4)-bicyclo[2.2.1]heptanacyclohexadecaphane

#### Phi-4.5. Numbering of heterophane parent hydrides with respect to heteroatoms described by skeletal replacement ('a') nomenclature

When there is a choice for numbering heterocyclic amplificants named by skeletal replacement nomenclature or for numbering simplified phane skeletons in which skeletal replacement has taken place, the following criteria are applied, in the order given, until a decision is reached.

*Phi-4.5.1.* Lowest locants are assigned to heteroatoms considered together without regard to the nature of the heteroatom, first with regard to the set of primary locants of the heteroatoms, i.e., the locants of the simplified skeleton (without including any superscript numbers), and then, if these locants are identical, with regard to the set of complete heteroatom locants, which includes the primary locant and superscript numbers (see also Phi-3.3.3).

## Example 26.



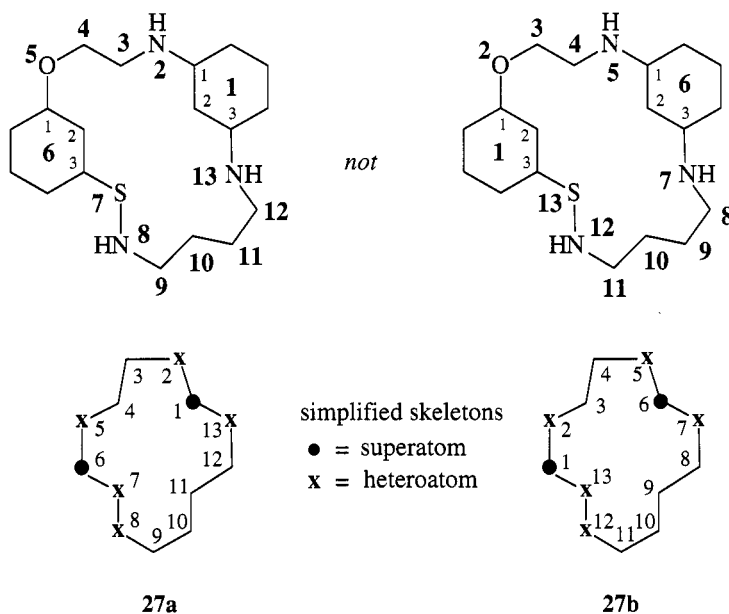
## Example 26. (cont'd)

Step 1: 1(2,5)-thiophena-5(1,3)-cyclohexanacyclooctaphane

Step 2: 2,7-dithia-1(2,5)-thiophena-5(1,3)-cyclohexanacyclooctaphane (26a)

not 3,8-dithia-1(2,5)-thiophena-5(1,3)-cyclohexanacyclooctaphane (26b) [the locant set for the heteroatoms in 26a, '2,7', is lower than the locant set in 26b, '3,8'.]

## Example 27.

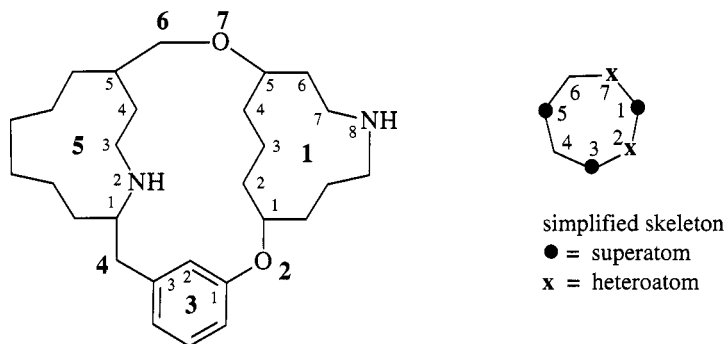


Step 1: 1,6(1,3)-dicyclohexanacyclotridecaphane

Step 2: 5-oxa-7-thia-2,8,13-triaza-1,6(1,3)-dicyclohexanacyclotridecaphane (27a)

not 2-oxa-13-thia-5,7,12-triaza-1,6(1,3)-dicyclohexanacyclotridecaphane (27b) (The locant set for all heteroatoms in 27a, '2,5,7,8,13', cited for comparison in ascending order, is lower than the locant set in 27b, '2,5,7,12,13'.)

## Example 28.

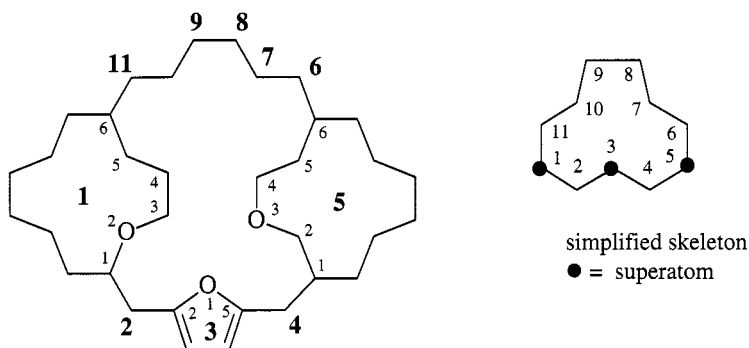


Step 1: 1,5(1,5)-dicycloundecana-3(1,3)-benzenacycloheptaphane

Step 2: 2,7-dioxa-1<sup>8</sup>,5<sup>2</sup>-diazia-1,5(1,5)-dicycloundecana-3(1,3)-benzenacycloheptaphane

not 4,6-dioxa-1<sup>2</sup>,5<sup>8</sup>-diazia-1,5(1,5)-dicycloundecana-3(1,3)-benzenacycloheptaphane (The primary locant set in the correct name, cited for comparison in ascending order, '1,2,5,7', is lower than the locant set '1,4,5,6'.)

## Example 29.



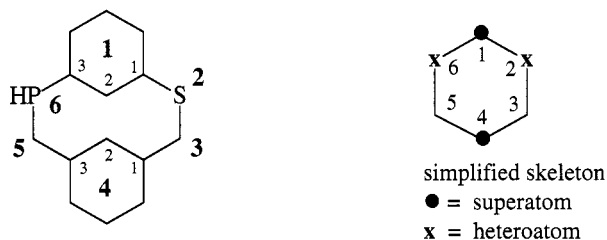
Step 1: 3(2,5)-furana-1,5(1,6)-dicyclododecanacycloundecaphane

Step 2: 1<sup>2</sup>,5<sup>3</sup>-dioxo-3(2,5)-furana-1,5(1,6)-dicyclododecanacycloundecaphane

not 1<sup>3</sup>,5<sup>2</sup>-dioxo-3(2,5)-furana-1,5(1,6)-dicyclododecanacycloundecaphane (The primary heteroatom locant sets are the same, '1,3,5'; the composite heteroatom locant set 1<sup>2</sup>,5<sup>3</sup> is lower than the locant set 1<sup>3</sup>,5<sup>2</sup>.)

*PhI-4.5.2.* Lowest locants are assigned to heteroatoms considered in the order of their priority, i.e., O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B (refs 1m,2m,19a), first with regard to the set of primary locants of the heteroatoms, i.e., the locants of the simplified skeleton (without including any superscript numbers), and then, if these locants are identical, with regard to the set of complete heteroatom locants, which includes the primary locant and superscript numbers (see also PhI-3.3.3).

## Example 30.

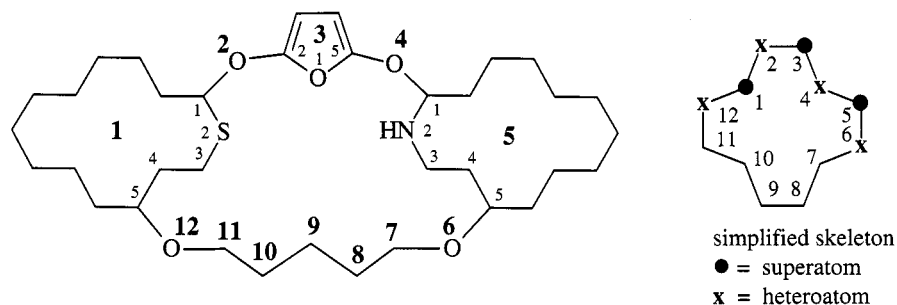


Step 1: 1,4(1,3)-dicyclohexanacyclonexaphane

Step 2: 2-thia-6-phospha-1,4(1,3)-dicyclohexanacyclonexaphane

not 6-thia-2-phospha-1,4(1,3)-dicyclohexanacyclonexaphane (Since thia is preferred to phospha in the element priority order, it must be given the lower locant.)

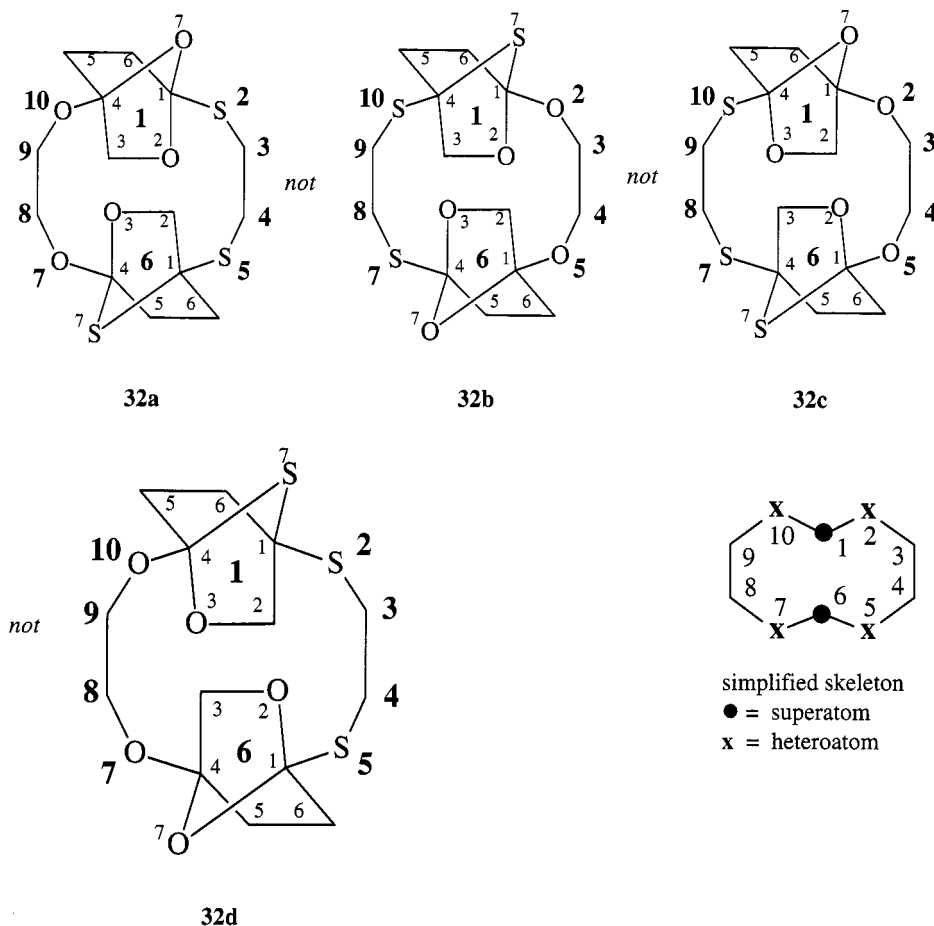
## Example 31.



Step 1: 3(2,5)-furana-1,5(1,5)-dicyclotetradecanacyclododecaphane

Step 2: 2,4,6,12-tetraoxa-1<sup>2</sup>-thia-5<sup>2</sup>-aza-3(2,5)-furana-1,5(1,5)-dicyclotetradecanacyclododecaphane  
*not* 2,4,6,12-tetraoxa-5<sup>2</sup>-thia-1<sup>2</sup>-aza-3(2,5)-furana-1,5(1,5)-dicyclotetradecanacyclododecaphane  
 (Application of PhI-4.5.1 reveals that both the primary locant sets and the locant sets including the composite locants for the heteroatoms without regard to the kind of heteroatom are the same for both names, 1,2,4,5,6,12 and 1<sup>2</sup>,2,4,5<sup>2</sup>,6,12, respectively. Since the primary locants for the 'oxa' prefixes are also the same, the primary locant for the next most senior heteroatom, 'thia', is compared and in the correct name the primary locant '1' is lower than the primary locant '5'.)

Example 32.



Step 1: 1,6(1,4)-dibicyclo[2.2.1]heptanacyclododecaphane

Step 2: 1<sup>2</sup>,1<sup>7</sup>,6<sup>3</sup>,7,10-pentaoxa-2,5,6<sup>7</sup>-trithia-1,6(1,4)-dibicyclo[2.2.1]heptanacyclododecaphane (32a)

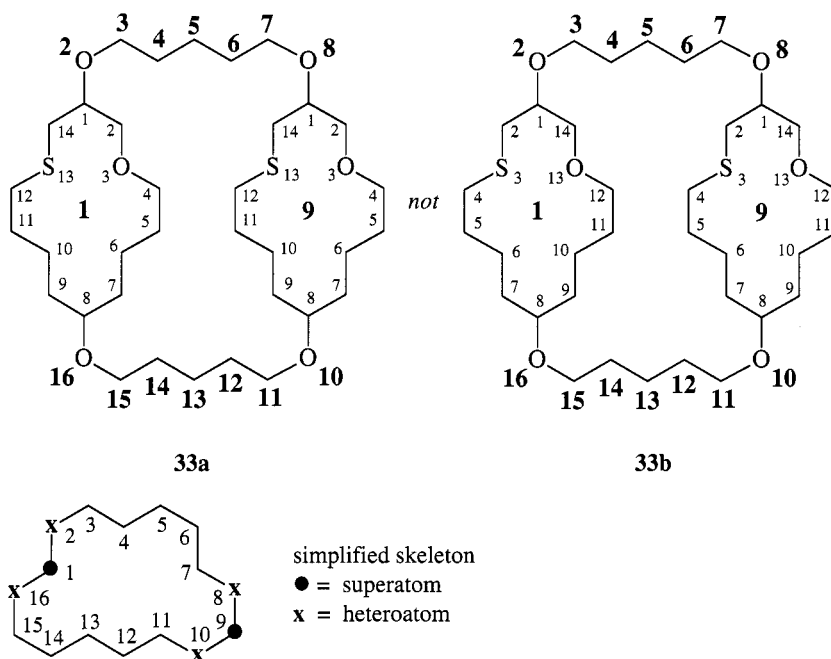
*not* 1<sup>2</sup>,2,5,6<sup>3</sup>,6<sup>7</sup>-pentaoxa-1<sup>7</sup>,7,10-trithia-1,6(1,4)-dibicyclo[2.2.1]heptanacyclododecaphane (32b)

*not* 1<sup>3</sup>,1<sup>7</sup>,2,5,6<sup>2</sup>-pentaoxa-6<sup>7</sup>,7,10-trithia-1,6(1,4)-dibicyclo[2.2.1]heptanacyclododecaphane (32c)

*not* 1<sup>3</sup>,6<sup>2</sup>,6<sup>7</sup>,7,10-pentaoxa-1<sup>7</sup>,2,5-trithia-1,6(1,4)-dibicyclo[2.2.1]heptanacyclododecaphane (32d)

(Application of PhI-4.5.1 eliminates names 32c and 32d because, although the primary locant sets for the heteroatoms, without regard to the kind of heteroatom, for 32a and 32b are the same, 1,1,2,5,6,6,7,10, the locant sets including composite locants for both, 1<sup>2</sup>,1<sup>7</sup>,2,5,6<sup>3</sup>,6<sup>7</sup>,7,10, are lower than the corresponding locant set for 32c and 32d, 1<sup>3</sup>,1<sup>7</sup>,2,5,6<sup>2</sup>,6<sup>7</sup>,7,10. Then, according to PhI-4.5.2, the name for 32a is correct because its set of primary locants for 'oxa', 1,1,6,7,10, is lower than the set of primary locants for 'oxa' in 32b, 1,2,5,6,6.)

## Example 33.



Step 1: 1,9(1,8)-dicyclotetradecanacyclohexadecaphane

Step 2:  $1^3,2,8,9^3,10,16$ -hexaoxa- $1^{13},9^{13}$ -dithia-1,9(1,8)-dicyclotetradecanacyclohexadecaphane (33a)

not  $1^{13},2,8,9^{13},10,16$ -hexaoxa- $1^3,9^3$ -dithia-1,9(1,8)-dicyclotetradecanacyclohexadecaphane (33b) (In both names the primary locant sets and the locant sets including the composite locants for the heteroatoms without regard to the kind of heteroatom, 1,1,2,8,9,9,10,16 and  $1^3,1^{13},2,8,9^3,9^{13},10,16$ , respectively, are the same. The primary locant sets for the senior prefix 'oxa' are also the same in both cases, 1,2,8,9,10,16, but for the locant sets including composite locants, the locant set for the prefix 'oxa' in 33a,  $1^3,2,8,9^3,10,16$ , is lower than the corresponding locant set for 'oxa' in 33b,  $1^{13},2,8,9^{13},10,16$ .)

## PHI-5. GUIDE TO CONSTRUCTION OF PHANE PARENT HYDRIDE NAMES

Construction of phane parent hydride names must follow the strict sequence of operations given below.

- Sort the heterocyclic amplificants into two types: (a) those that can be named as heterocycles (following points 2–7) without the use of skeletal replacement ('a') nomenclature; and (b) those that are named using skeletal replacement ('a') nomenclature. The latter must be named as hydrocarbons (following points 2–7) and modified at point 8 by replacement ('a') nomenclature.
- Simplify the phane parent hydride to arrive at the simplified phane skeleton.
- Number the simplified phane skeleton giving priority to superatoms for lowest locants.
- Name and number the amplificants, respecting point 1, above, and the principle of lowest locants.
- Name the phane parent hydride provided that no choices have to be made regarding the numbering of the simplified phane skeleton or amplificants.
- Choose the numbering for symmetrical simplified phane skeletons according to the following criteria applied in sequence until no further choice is necessary:
  - seniority order of amplificants;
  - amplificants with lowest locants;

- c. lowest amplificant locants compared in order of the increasing value of their respective superatom locants.
7. Number the phane parent hydride as a whole.
  8. Apply the principles of skeletal replacement ('a') phane nomenclature to generate a heterocyclic phane parent hydride.

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