

IR-6 Parent Hydride Names and Substitutive Nomenclature (Draft March 2004)

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IR-6.1 INTRODUCTION

Substitutive nomenclature is a system in which names are based on names of *parent hydrides* implying a defined standard population of hydrogen atoms attached to a skeletal structure. Names of *derivatives* of the parent hydrides are formed by citing suffixes or prefixes appropriate to the *substituent groups* (or *substituents* for short) replacing the hydrogen atoms (preceded by locants when required), joined without a break to the name of the unsubstituted parent hydride.

Substitutive nomenclature is recommended only for derivatives of the parent hydrides named in Table IR-6.1 (see below), and derivatives of polynuclear hydrides containing only these elements (see Sections IR-6.2.2 - IR-6.2.4). The bonding numbers of the skeletal atoms are understood to be as in the Table (these bonding numbers, *e.g.* 4 for Si and 2 for Se, are termed *standard bonding numbers*). Other bonding numbers must be indicated by an appropriate designator (the ' λ convention', see Section IR-6.2.2.2 and Section P-14.1.3 of Ref. 1).

In general, relevant practices and conventions of substitutive nomenclature as applied to organic compounds¹ are also followed here.

Constructing a substitutive name involves the replacement of hydrogen atoms in a parent structure with other atoms or atom groups. Related operations, often considered to be part of substitutive nomenclature, are *skeletal replacement* (Section IR-6.2.4.1) and *functional replacement* in oxoacid parents (Section IR-8.6). In most cases, the compounds named substitutively in the present chapter may alternatively and equally systematically be named additively (Chapter IR-7), but it is important to note that for the parent hydrides presented here such additive names cannot be used as *parent names* in substitutive nomenclature.

Neutral boron hydrides are called boranes. The basic aspects of borane nomenclature are provided in Section IR-6.2.3; more advanced aspects will be treated in a future IUPAC publication.

IR-6.2 PARENT HYDRIDE NAMES

IR-6.2.1 **Mononuclear parent hydrides with standard and non-standard bonding numbers**

The mononuclear hydrides of elements of groups 13-17 of the Periodic Table play a central role in substitutive nomenclature. They are used as parent hydrides as indicated above with the parent names given in Table IR-6.1.

Table IR-6.1 Parent names of mononuclear hydrides

(Insert separate landscape Table)

In cases where the bonding number deviates from the standard number defined above, it must be indicated in the hydride name by means of an appropriate superscript appended to the Greek letter λ , this symbol being separated from the name in Table IR-6.1 by a hyphen.

Examples:

1. PH_5 λ^5 -phosphane
2. PH λ^1 -phosphane
3. SH_6 λ^6 -sulfane
4. SnH_2 λ^2 -stannane

IR-6.2.2 **Homopolynuclear parent hydrides (other than boron and carbon hydrides)**IR-6.2.2.1 *Homonuclear acyclic parent hydrides in which all atoms have their standard bonding number*

Names are constructed by prefixing the 'ane' name of the corresponding mononuclear hydride from Table IR-6.1 with the appropriate multiplicative prefix ('di', 'tri', 'tetra', etc. see Table IV*) corresponding to the number of atoms of the chain bonded in series.

Examples:

1. HOOH dioxidane, or hydrogen peroxide
2. H_2NNH_2 diazane, or hydrazine
3. H_2PPH_2 diphosphane
4. H_3SnSnH_3 distannane
5. HSeSeSeH triselane
6. $\text{SiH}_3\text{SiH}_2\text{SiH}_2\text{SiH}_3$ tetrasilane

* Tables numbered with a Roman numeral are collected together at the end of this book.

The compositional name 'hydrogen peroxide' (*cf.* Chapter IR-5) is an alternative to 'dioxidane' for H_2O_2 itself, but is not applicable as a parent hydride name in substitutive nomenclature.

In Section P-68.3.1.2.1 of Ref. 1 organic derivatives of H_2NNH_2 are named on the basis of 'hydrazine' as a parent name.

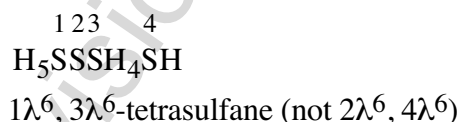
IR-6.2.2.2 *Homonuclear acyclic parent hydrides with elements exhibiting non-standard bonding numbers*

In cases where the skeletal atoms of a hydride chain are the same but one or more has a bonding number different from the standard values defined by Table IR-6.1, the name of the hydride is formed as if all the atoms showed standard bonding numbers, but is preceded by locants, one for each non-standard atom, each locant qualified without a space by λ^n , where n is the appropriate bonding number.

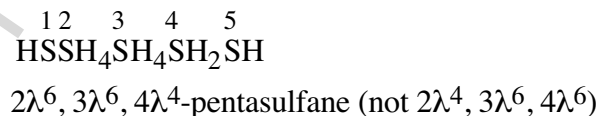
When a choice is needed between the same skeletal atom in different valence states, the one in a non-standard valence state is preferred for assignment of the lower locant. If a further choice is needed between the same skeletal atom in two or more non-standard valence states, preference for the lower locant or locants is given in order of decreasing numerical value of the bonding number, *i.e.* λ^6 is preferred to λ^4 .

Examples:

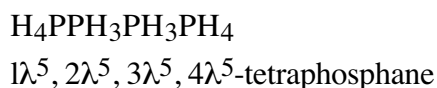
1.



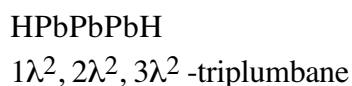
2.



3.



4.



IR-6.2.2.3 *Unsaturated homonuclear acyclic hydrides*

Chains containing unsaturation are accommodated in substitutive nomenclature by the methods used with alkenes and alkynes (see Section P-31.1 of Ref. 1), *i.e.* the name of the corresponding saturated chain hydride is modified by replacing the 'ane' suffix with 'ene' in the case of a double bond and 'yne' in the case of a triple bond. If there is one of each, the suffix becomes 'en' ...'yne' with appropriate locants; 'diene' is used when there are two double bonds, and so on. In each case the position(s) of unsaturation is/are indicated by (a) numerical locant(s) *immediately* preceding the suffix(es). Locants are chosen to be as low as possible.

Examples:

- | | | |
|----|--|--|
| 1. | HN=NH | diazene |
| 2. | HSb=SbH | distibene |
| 3. | $\begin{array}{cccc} 1 & 2 & 3 & 4 & 5 \\ \text{H}_2 & \text{NN} & = & \text{NH} & \text{NNH}_2 \end{array}$ | pentaaz-2-ene (not pentaaz-3-ene,
and not pentaz-2-ene) |

Unsaturated acyclic hydrides are not classified as parent hydrides. Because of the hierarchical rules of substitutive nomenclature, the numbering of the double and triple bonds may not be fixed until various groups and modifications with higher priority have been numbered. (See Section IR-6.4.9 for an example).

IR-6.2.2.4 *Homonuclear monocyclic parent hydrides*

There are three main ways of giving parent names to homonuclear monocyclic hydrides:

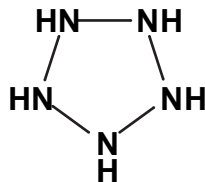
- (i) by using the Hantzsch-Widman (H-W) name (see Section IR-6.2.4.3 and Section P-22.2.2 of Ref. 1);
- (ii) by using the relevant replacement prefix ('a' term) from Table X together with the appropriate multiplicative prefix to indicate replacement of carbon atoms in the corresponding carbocyclic compound;
- (iii) by adding the prefix 'cyclo' to the name of the corresponding unbranched, unsubstituted chain (see Sections IR-6.2.2.1 - IR-6.2.2.3 and Section P-22.2.4 of Ref. 1).

Each method is used in Examples 1-4 below. When naming organic derivatives of non-carbon homonuclear monocyclic parent hydrides, the Hantzsch-Widman name is preferred

for rings with 3 to 10 members. For larger rings, the names given by the second method are preferred.

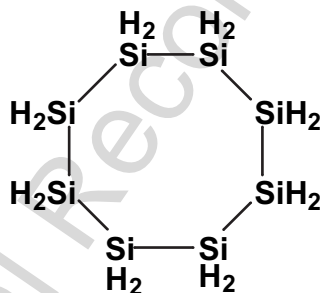
Examples:

1.



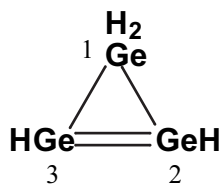
- (i) H-W name: pentazolidine
- (ii) pentaazacyclopentane
- (iii) cyclopentaazane

2.



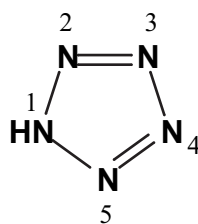
- (i) H-W name: octasilocane
- (ii) octasilacyclooctane
- (iii) cyclooctasilane

3.

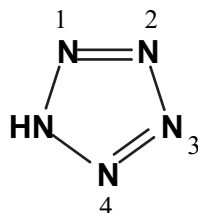


- (i) H-W name: 1*H*-trigermirene
- (ii) trigermacyclopropene
- (iii) cyclotrigermene

4.



(i) H-W name: 1*H*-pentazole



(ii) pentaazacyclopenta-1,3-diene

(iii) cyclopentaaza-1,3-diene

Note that in Example 4 the numbering for the H-W name differs from that for the other two methods; H-W priorities depend on the H-atom position, and those in (ii) and (iii) on the locations of the double bonds.

IR-6.2.2.5 *Homonuclear polycyclic parent hydrides*

Parent names of homonuclear polycycles may be constructed by any one of three methods:

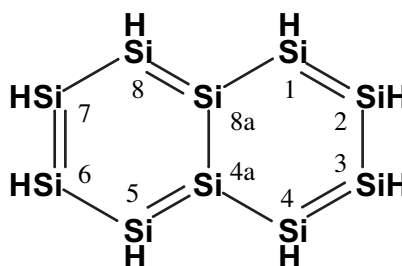
(i) by specifying the fusion of relevant monocycles (Section P-25.3.2 of Ref. 1), each named by the Hantzsch-Widman system (see Section IR-6.2.4.3);

(ii) using a skeletal replacement prefix ('a' term) from Table X together with the appropriate multiplicative prefix to indicate replacement of the carbon atoms in the corresponding carbocyclic compound;

(iii) specifying the ring structure using the von Baeyer notation (Section P-23.4 of Ref. 1) in combination with the name of the corresponding linear hydride as derived in Section IR-6.2.2.1.

Examples:

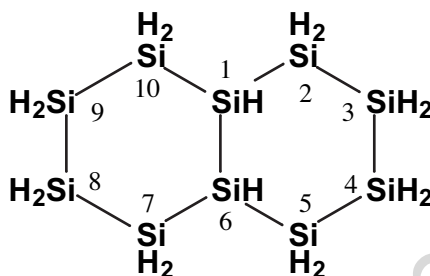
1.



(i) hexasilinohexasiline

(ii) decasilanaphthalene

2.



(iii) bicyclo[4.4.0]decasilane

(von Baeyer name)

IR-6.2.3 Boron hydrides

IR-6.2.3.1 Stoichiometric names

Neutral polyboron hydrides are called boranes and the simplest possible parent structure, BH_3 , is given the name 'borane'. The number of boron atoms in a boron hydride molecule is indicated by a numerical prefix. The principal difference between this system of naming and hydrocarbon nomenclature is that the number of hydrogen atoms must be defined; it cannot be inferred from simple bonding considerations. The number of hydrogen atoms is indicated by the appropriate arabic numeral in parentheses directly following the name. Such names convey only compositional information.

Examples:

1. B_2H_6 diborane(6)
2. $\text{B}_{20}\text{H}_{16}$ icosaborane(16)

IR-6.2.3.2 Structural descriptor names

More structural information is obtained by augmenting the stoichiometric name by a structural descriptor. The descriptor is based on electron-counting relationships⁴ and is presented in Table IR-6.2.

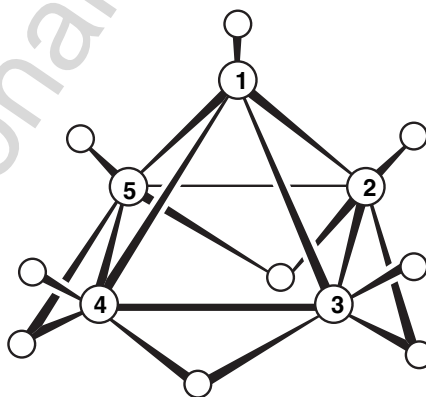
Table IR-6.2. Summary of common polyboron hydride structure types according to stoichiometry and electron-counting relationships.

Descriptor	Skeletal electron pairs	Parent hydride	Description of structure
<i>closo</i>	$n+1$	B_nH_{n+2}	Closed polyhedral structure with triangular faces only.
<i>nido</i>	$n+2$	B_nH_{n+4}	Nest-like non-closed polyhedral structure; n vertices of the parent $(n+1)$ -atom <i>closo</i> polyhedron occupied.
<i>arachno</i>	$n+3$	B_nH_{n+6}	Web-like non-closed polyhedral structure; n vertices of the parent $(n+2)$ -atom <i>closo</i> polyhedron occupied.
<i>hypho</i>	$n+4$	B_nH_{n+8}	Net-like non-closed polyhedral structure; n vertices of the parent $(n+3)$ -atom <i>closo</i> polyhedron occupied.
<i>klado</i>	$n+5$	B_nH_{n+10}	Open branch-like polyhedral structure; n vertices of the parent $(n+4)$ -atom <i>closo</i> polyhedron occupied.

(The structural relationships are often represented by a Rudolph diagram.⁵)

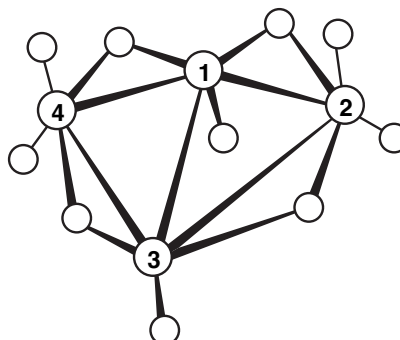
Examples:

1.



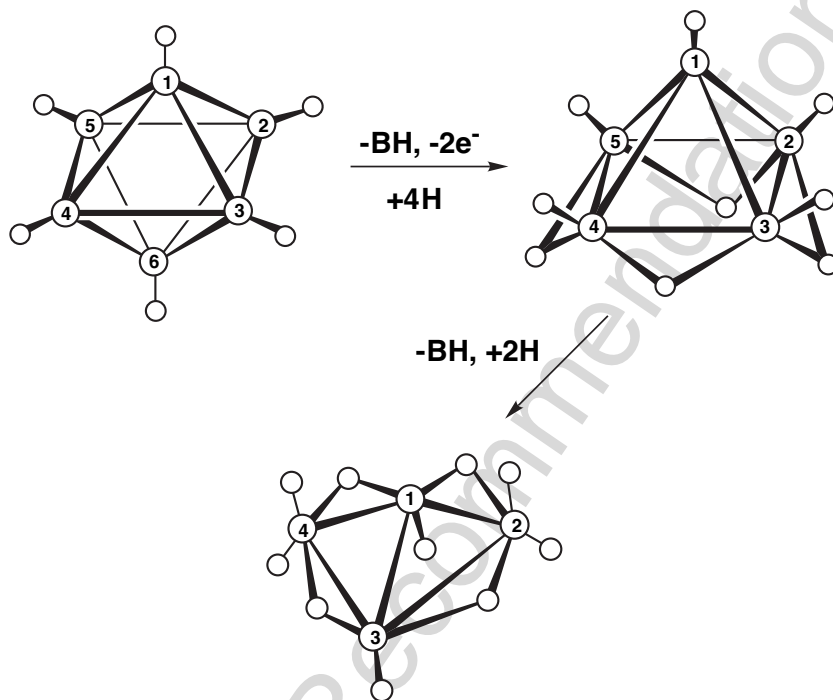
nido-pentaborane(9), B_5H_9

2.



arachno-tetraborane(10), B₄H₁₀

The two structures in Examples 1 and 2 can be thought of as related to that of *closo*-B₆H₆²⁻ as follows:



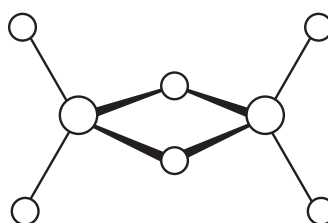
The structures are obtained formally by removal of one (Example 1) or two (Example 2) BH groups from, and the addition of the appropriate number of electrons and hydrogen atoms to, the highest connectivity vertices of *closo*-B₆H₆²⁻.

It should be noted that the prefixes *nido*, *arachno*, *etc.* are not used for the simplest boranes for which formal derivation from *closo* parent structures by successive subtractions might seem to be far-fetched.

Chain compounds may be explicitly specified as such by using the prefix '*catena*'.

Examples:

3.

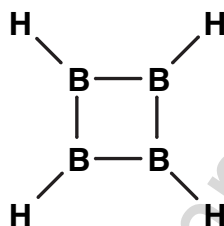


diborane(6), B₂H₆

4. H_2BBHBH_2 *catena-triborane*(5)
5. $\text{HB}=\text{BBH}_2$ *catena-triborene*(3)

For cyclic systems, the prefix 'cyclo' in connection with the name of the corresponding chain compound or the Hantzsch-Widman (H-W) nomenclature system (*cf.* Section IR-6.2.4.3) may be used.

6.



cyclotetraborane

H-W name: tetraboretane

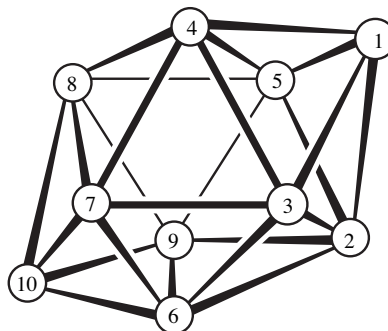
IR-6.2.3.3 *Systematic numbering of polyhedral clusters*

It is necessary to number the boron skeleton for each cluster systematically, so as to permit the unambiguous naming of the substituted derivatives. For this purpose, the boron atoms of *closo* structures are considered as occupying planes disposed sequentially, perpendicular to the axis of highest order symmetry. (If there are two such axes, the 'longer', in terms of the greater number of perpendicular planes crossed, is chosen).

Numbering begins at the nearest boron atom when the cluster is viewed along this axis and proceeds either clockwise or anti-clockwise, dealing with all skeletal atoms of the first plane. Numbering then continues in the same sense in the next plane, beginning with the boron atom nearest to the lowest numbered boron atom in the preceding plane when going forward in the direction of numbering.

Example:

1.

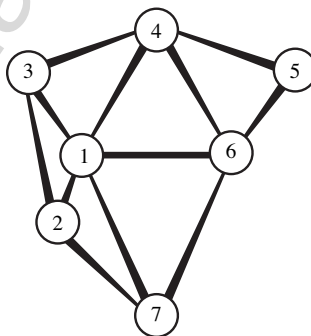


closo-B₁₀H₁₀²⁻ (hydrogen atoms omitted for clarity)

The numbering in *nido* clusters is derived from that of the related *closo* cluster. In the case of *arachno* and more open clusters, the opened side is presented towards the observer and the boron atoms considered as projected onto a plane at the rear. They are then numbered sequentially in zones, commencing at the central boron atom of highest connectivity and proceeding clockwise or anti-clockwise until the innermost zone is completed. The next zone is then numbered in the same sense starting from the 12 o'clock position, and so on until the outermost zone is completed. This treatment means that the numbering of the *closo* parent is unlikely to carry over into the corresponding *arachno* system.

Examples:

2.



arachno-B₇H₁₃ (hydrogen atoms omitted for clarity)

When there is a choice, the molecule is so oriented that the 12 o'clock position is decided by sequential application of the following criteria:

(i) the 12 o'clock position lies in a symmetry plane, which contains as few boron atoms as possible;

(ii) the 12 o'clock position lies in that portion of the symmetry plane which contains the greatest number of skeletal atoms;

(iii) the 12 o'clock position lies opposite the greater number of bridging atoms.

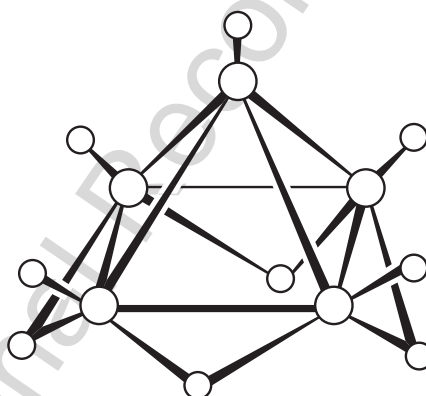
The use of criteria (i)-(iii) may fail to effect a decision, and where a symmetry plane is lacking they are inapplicable. In such cases the general principles of organic numbering are used, such as choosing a numbering scheme which gives substituted atoms the lowest locants.

IR-6.2.3.4 *Systematic naming giving hydrogen atom distribution*

In open boranes each boron atom can be assumed to carry at least one terminal hydrogen atom. However, it is necessary to specify the positions of the bridging hydrogen atoms by using the symbol μ , preceded by the locants for the skeletal positions so bridged in ascending numerical order. The designator *H* is used for the bridging hydrogen atoms in the name.

Example:

1.



2,3:2,5:3,4:4,5-tetra- μH -nido-pentaborane(9)

This method of locating bridging hydrogen atoms is adapted from the 'indicated hydrogen' method in organic nomenclature (see Section P-14.6 of Ref. 1). The 'indicated hydrogen' method would yield the name (2,3- μH),(2,5- μH),(3,4- μH),(4,5- μH)-nidopentaborane(9).

IR-6.2.4 **Heteronuclear parent hydrides**

IR-6.2.4.1 *Heteronuclear acyclic parent hydrides in general*

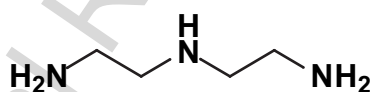
When at least four carbon atoms in an unbranched-chain parent hydrocarbon are replaced by heteroatoms, alike or different, and the terminal carbon atoms either remain or are replaced by P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, or Tl, *skeletal replacement nomenclature* ('a' nomenclature) may be used to indicate the heteroatoms (see Section P-15.4 of Ref. 1).

In this method, the chain is named first as if it were composed entirely of carbon atoms. Any heteroatoms in the chain are then designated by appropriate replacement prefixes ('a' terms) from Table X cited in the priority order given by Table VI, each preceded by its appropriate locant. The locants are assigned by numbering the chain from that end which gives lower locants to the heteroatom set as a whole and, if these are equal, from that end which gives the lower locant or locant set to the replacement prefix first cited. If there is still a choice, lower locants are assigned to the sites of unsaturation.

Only chains with four or more heteroatoms (or strictly speaking, four or more *heterounits*) are given parent names constructed in this way. A heterounit is a sequence of heteroatoms which is in itself the skeleton of a parent hydride, *e.g.* SS and SiOSi (*cf.* Section IR-6.2.4.2) but not OSiO. Heteroatoms must not belong to the principal characteristic group (see Section IR-6.3.1) (if there is one) when counting them for this purpose. Heteronuclear chains with fewer heterounits, and heteronuclear chains not terminating in any of the atoms listed above, are named substitutively as derivatives of homonuclear parent hydrides and are not themselves used as parents.

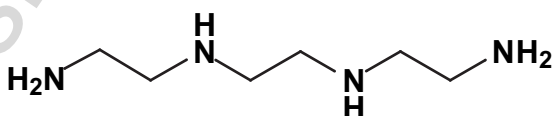
Examples:

1.



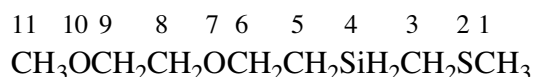
N-(2-aminoethyl)ethane-1,2-diamine

2.



N,N-bis(2-aminoethyl)ethane-1,2-diamine

3.



7,10-dioxa-2-thia-4-silaundecane

(Parent name. Note the name is not 2,5-dioxa-10-thia-8-silaundecane because the locant set 2,4,7,10 takes precedence over the locant set 2,5,8,10)

Unambiguous parent names for non-carbon-containing heteronuclear chains can be derived from a hydrocarbon parent or a non-carbon homonuclear chain parent (*cf.* Section IR-6.2.2.1). Alternatively, heteronuclear chains may be named additively by the method described in Section IR-7.4. However, such names cannot be used as parent names in substitutive nomenclature.

Example:

4.



1,2,3,5-tetrasil-4-germapentane (not 1,3,4,5-tetrasil-2-germapentane),

or 2-germapentasilane, or

1,1,1,2,2,3,3,4,4,5,5,5-dodecahydrido-2-germy-1,2,3,5-tetrasilyl-[5]catena

IR-6.2.4.2 *Hydrides consisting of chains of alternating skeletal atoms*

Chains hydrides with a backbone of alternating atoms of two elements A and E, neither of which is carbon, *i.e.* of sequences $(\text{AE})_n\text{A}$, where element A occurs later in the sequence of Table VI, can be named by successive citation of the following name parts:

(i) a numerical prefix (Table IV) denoting the number of atoms of element A, with no elision of a terminal vowel of this prefix;

(ii) replacement prefixes ending in 'a' (Table X) denoting elements A and E in that order (with elision of the terminal 'a' of the replacement prefix before another 'a' or an 'o');

(iii) the ending 'ne'.

Examples:

1.	$\text{SnH}_3\text{OSnH}_2\text{OSnH}_2\text{OSnH}_3$	tetrastannoxane
2.	$\text{SiH}_3\text{SSiH}_2\text{SSiH}_2\text{SSiH}_3$	tetrasilathiane
3.	$\text{PH}_2\text{NHPHNHPH}_2$	triphosphazane
4.	$\text{SiH}_3\text{NHSiH}_3$	disilazane
5.	$\text{PH}_2\text{N}=\text{PNHPHNHPH}_2$	tetraphosphaz-2-ene

The first four structures are parent hydrides, but not the unsaturated compound (*cf.* remarks in Section IR-6.2.2.3).

IR-6.2.4.3 *Heteronuclear monocyclic parent hydrides; Hantzsch-Widman nomenclature*

For heteronuclear monocyclic parent hydrides there are two general naming systems and, in certain cases, a third possibility.

(i) In the (extended) Hantzsch-Widman (H-W) system (Section P-22.2.2 of Ref. 1), names are constructed so as to convey the ring size, the presence of heteroatoms (*i.e.* non-carbon atoms) and the degree of hydrogenation (either *mancude*, *i.e.* with the maximum number of non-cumulative double bonds, or saturated) by means of characteristic endings. These endings are given in Table IR-6.3. (Hydrides with intermediate degrees of hydrogenation are named by the use of the prefix 'hydro' together with an appropriate multiplicative prefix. However, such hydrides are not parents.)

The order of citation of the heteroatoms follows Table VI, *i.e.* F > Cl > Br > I > O > ...*etc.*, where '>' means 'is cited before'. Locants are assigned to the heteroatoms so as to ensure first that the locant '1' is given to the atom cited first and then that the total set of locants is as low as possible consistent with sequential numbering of the ring positions (ordering locant sets lexicographically). The heteroatoms are cited by the replacement prefixes ('a' terms) given in Table X together with appropriate multiplicative prefixes. In the case of six-membered rings, the ring heteroatom which is cited last decides which of the alternative endings in Table IR-6.3 is chosen.

Tautomers may be distinguished using indicated hydrogen to specify the location of the hydrogen atom(s) which can be placed in several ways [and thus, indirectly, the location of the double bond(s)], as in Example 2 below.

Table IR-6.3 Endings in the Hantzsch-Widman system

<i>Number of atoms in ring</i>	<i>Mancude</i> ^a	<i>Saturated</i>
3	irene ('irine' for rings with N as only heteroatom)	irane ('iridine' for rings containing N)
4	ete	etane ('etidine' for rings containing N)
5	ole	olane ('olidine' for rings containing N)
6(A) ^b	ine	ane
6(B) ^b	ine	inane
6(C) ^b	inine	inane
7	epine	epane

8	ocine	ocane
9	onine	onane
10	ecine	ecane

^a Maximum number of non-cumulative double bonds.

^b 6(A) is used when the last-cited heteroatom is O, S, Se, Te, Po, or Bi; 6(B) is used when the last-cited heteroatom is N, Si, Ge, Sn, or Pb; and 6(C) is used when the last-cited heteroatom is F, Cl, Br, I, P, As, Sb, B, Al, Ga, In, or Tl.

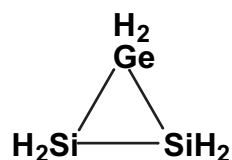
(ii) Alternatively, the name is based on the name of the corresponding carbocycle, and the heteroatoms are indicated by the replacement prefixes ('a' terms) from Table X together with appropriate multiplicative prefixes. The order of citation is again given by Table VI.

(iii) For the special case of rings of two alternating skeletal atoms (as in Examples 3-8 below), the name is constructed using the prefix 'cyclo' followed by the replacement prefixes (Table X) cited in the reverse of the order in which the corresponding elements appear in Table VI. The name ends with 'ane' if the repeating unit is saturated.

Method (ii) is only recommended for saturated rings and mancude rings (rings with the maximum number of non-cumulative double bonds) and method (iii) only for saturated rings. The Hantzsch-Widman names are preferred for rings with up to 10 members and method (ii) is preferred for saturated rings with more than 10 members. For more rules on large rings, see Section P-22.2.3 of Ref. 1.

Examples:

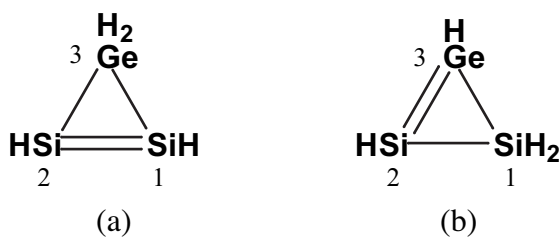
1.



(i) H-W name: disilagermirane

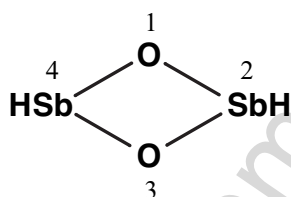
(ii) disilagermacyclopropane

2.



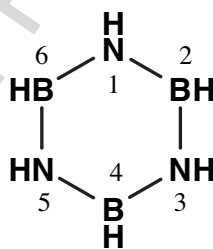
H-W names: *3H*-1,2,3-disilagermirene (a), and *1H*-1,2,3-disilagermirene (b)

3.



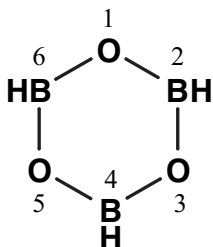
- (i) H-W name: 1,3,2,4-dioxadistibetane
 (ii) 1,3-dioxa-2,4-distibacyclobutane
 (iii) cyclodistiboxane

4.



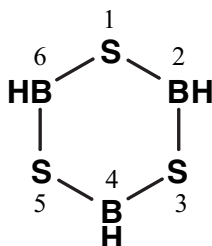
- (i) H-W name: 1,3,5,2,4,6-triazatriborinane
 (ii) 1,3,5-triaza-2,4,6-triboracyclohexane
 (iii) cyclotriborazane

5.



- (i) H-W name: 1,3,5,2,4,6-trioxatriborinane
 (ii) 1,3,5-trioxa-2,4,6-triboracyclohexane
 (iii) cyclotriboroxane

6.

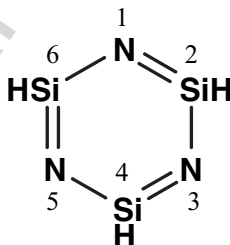


- (i) H-W name: 1,3,5,2,4,6-trithiatriborinane
 (ii) 1,3,5-trithia-2,4,6-triboracyclohexane
 (iii) cyclotriborathiane

The names borazole, boroxole and borthiole, respectively, for the three compounds in Examples 4, 5 and 6 have been abandoned long ago as they imply five-membered rings in the Hantzsch-Widman system. The names borazin(e), boroxin and borthiin indicate six-membered rings with unsaturation and only one boron atom and one other heteroatom (although the order of the element name stems is wrong) and are also not recommended.

Example:

7.

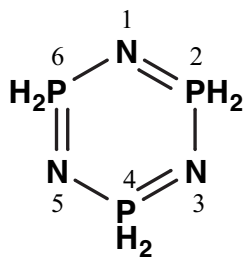


- (i) H-W name: 1,3,5,2,4,6-triazatrisiline
 (ii) 1,3,5-triaza-2,4,6-trisilacyclohexa-1,3,5-triene

Where ring atoms have a connectivity different from their standard bonding number (see Section IR-6.2.1), their actual bonding number is expressed as an arabic superscript to the Greek letter lambda following immediately after an appropriate locant.

Example:

8.



- (i) H-W name: 1,3,5,2 λ^5 , 4 λ^5 , 6 λ^5 -triazatriphosphinine
 (ii) 1,3,5-triaza-2 λ^5 , 4 λ^5 , 6 λ^5 -triphosphacyclohexa-1,3,5-triene

IR-6.2.4.4 Skeletal replacement in boron hydrides

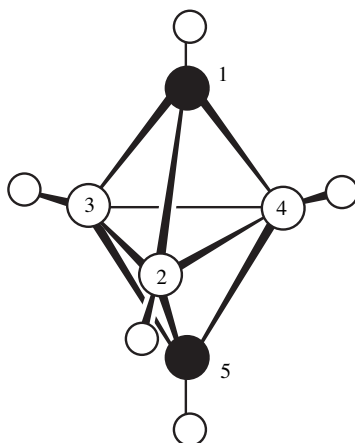
It is possible that the essential skeletal structure of the boron hydrides is preserved in derivatives in which one or more of the boron atoms are replaced by other atoms. The names of such species are formed by an adaptation of replacement nomenclature, giving carbaboranes, azaboranes, phosphaboranes, thiaboranes, *etc.*

In the heteroboranes, the number of nearest neighbours to the heteroatom is variable and can be 5, 6, 7, *etc.* Therefore, in the adaptation of replacement nomenclature to polyborane compounds, the replacement of a boron atom by another atom is indicated in the name along with the number of hydrogen atoms in the resulting polyhedral structure. The prefixes *closo*, *nido*, *arachno*, *etc.*, are retained as described for boron hydrides (Section IR-6.2.3.2). The positions of the supplanting heteroatoms in the polyhedral framework are indicated by locants which are the lowest possible numbers taken as a set consistent with the numbering of the parent polyborane. If a choice remains for locant assignment within a given set, then priority for low numbering should be assigned to the element encountered first using Table VI.

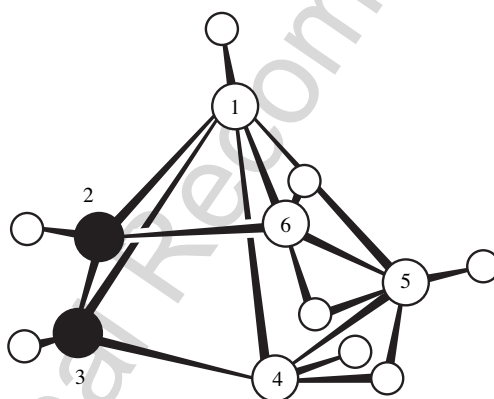
The hydrogen atom population of the actual compound concerned (and not that of the parent all-boron skeletal compound) is added as an arabic numeral in parentheses at the end of the name. The numeral is retained in hydrogen substitution.

Examples:

1. $B_{10}C_2H_{12}$ dicarba-*closo*-dodecaborane(12)
2. $B_3C_2H_5$ 1,5-dicarba-*closo*-pentaborane(5)



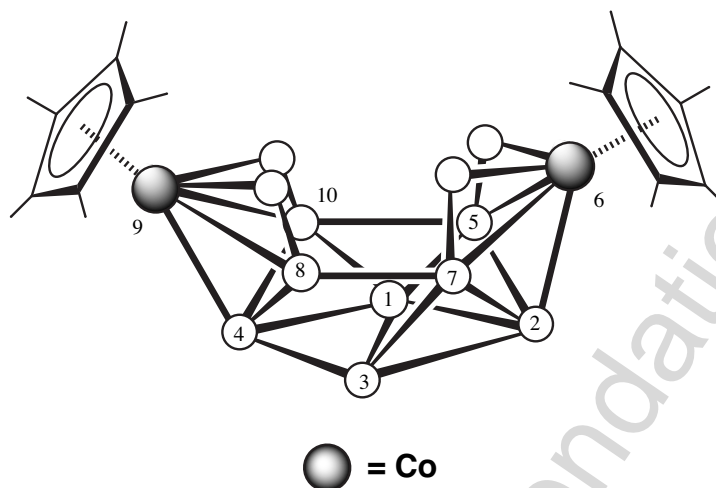
3. $B_4C_2H_8$ 4,5:5,6-di- μH -2,3-dicarba-*nido*-hexaborane(8)



Note that locants for skeletal replacement take precedence over those for bridging hydrogen atoms. The number of bridging hydrogen atoms is usually different for heteroboranes compared with parent polyboranes, and for numbering purposes only the symmetry of the parent boron skeleton is considered.

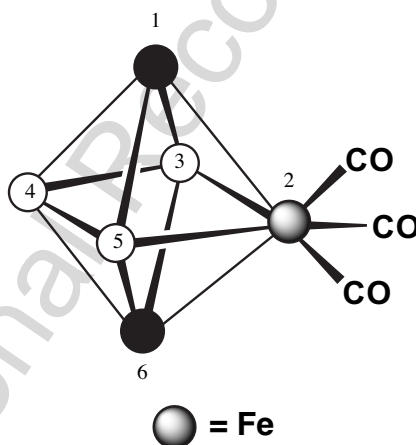
Examples:

4.



6,9-bis(η^5 -pentamethylcyclopentadienyl)-5,6:6,7:8,9:9,10-tetra- μH -6,9-dicobaltanido-decaborane(12) (one terminal hydrogen on each boron atom omitted for clarity).

5.



2,2,2-tricarbonyl-1,6-dicarbonyl-2-ferrocene-closo-hexaborane(5)

IR-6.2.4.5 Heteronuclear polycyclic parent hydrides

Parent names of heteronuclear polycycles may be constructed by three methods:

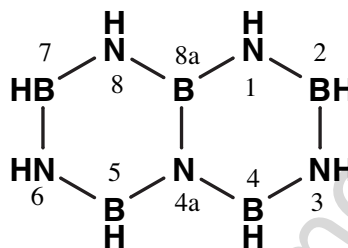
(i) specifying the fusion of relevant monocycles (see Section P-25.3.2 of Ref. 1), named by the Hantzsch-Widman system (see Section IR-6.2.4.3);

(ii) using replacement prefixes ('a' terms) from Table X to specify replacement of carbon atoms in the corresponding carbocyclic compound. Heteroatoms are cited in the order given by Table VI and appropriate multiplicative prefixes are added;

(iii) for ring systems consisting of repeating units, using the von Baeyer notation to specify the ring structure combined with the appropriate multiplicative prefix and the replacement prefixes from Table X appropriate to the repeating unit, *cf.* the names discussed in Section IR-6.2.4.2.

Example:

1.



{Numbering is only for method (ii)}

(i): octahydro[1,3,5,2,4,6]triazatriborinino[1,3,5,2,4,6]triazatriborinine

(ii): octahydro-1,3,4a,6,8-pentaaza-2,4,5,7,8a-pentaboranaphthalene

(iii): bicyclo[4.4.0]pentaborazane

In this example, names (i) and (ii) need the additional 'octahydro' prefixes because the available parent hydrides for these constructions (triazatriborinine and naphthalene, respectively) are mancude (*i.e.* have the maximum number of non-cumulative double bonds).

IR-6.3 SUBSTITUTIVE NAMES OF DERIVATIVES OF PARENT HYDRIDES

IR-6.3.1 Use of suffixes and prefixes

Substituent groups (or substituents), considered as replacing hydrogen atoms in parent hydrides, are named using appropriate suffixes ('ol', 'thiol', 'peroxol', 'carboxylic acid', *etc.*) and prefixes ('hydroxy', 'phosphanyl', 'bromo', 'nitro', *etc.*). Substituent suffixes are ranked, and suffixes and prefixes extensively listed, in Appendices 1 and 2 of Ref. 1. The case of substituents formed by removal of one or more hydrogen atoms from a parent hydride is explained briefly, with examples, in Section IR-6.4.7, and suffixes and prefixes for many common inorganic substituents are included in Tables III and IX, respectively.

Some substituents are always cited as prefixes, most notably halogen atoms. Otherwise, the highest-ranking substituent (the principal characteristic group) is cited as a suffix and the rest of the substituents as prefixes. Except for 'hydro', prefixes are cited in alphabetical order before the name of the parent hydride, parentheses being used to avoid ambiguity.

Multiplicative prefixes indicate the presence of two or more identical substituents; if the substituents themselves are substituted, the prefixes 'bis', 'tris', 'tetrakis', *etc.* are used. In the case of a multiplicative prefix ending in 'a' and a suffix starting with a vowel, the 'a' is elided (see Example 2 below). The final 'e' of a parent hydride name is elided in front of a suffix starting with a vowel (see Examples 1 and 6 below).

Where there is a choice of parent hydride among those listed in Table IR-6.1 (or corresponding hydrides with non-standard bonding numbers, *cf.* Section IR-6.2.2.2), the name is based on the parent hydride of the element occurring first in the sequence: N, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, Tl, O, S, Se, Te, C, F, Cl, Br, I.

The above exposition is only a very brief overview of the most important principles of substitutive nomenclature. In Ref. 1, an extensive system of rules is developed for choosing one name among the many unambiguous substitutive names that may often be constructed for organic compounds. A corresponding extensive set of rules has not been developed for non carbon-containing compounds, partly because many such compounds can just as well be given additive names (Chapter IR-7), and often are.

The following names exemplify the above principles. In some cases, additive names are given for comparison.

Examples:

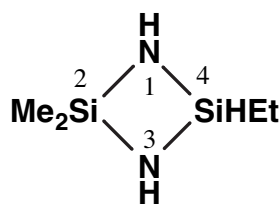
- | | | |
|-----|--|--|
| 1. | SiH ₃ OH | silanol |
| 2. | S(OH) ₂ | sulfanediol (substitutive),
or dihydroxidosulfur (additive) |
| 3. | SF ₆ | hexafluoro-λ ⁶ -sulfane (substitutive),
or hexafluoridosulfur (additive) |
| 4. | TIH ₂ CN | thallanecarbonitrile (substitutive),
or cyanidodihydridthallium (additive) |
| 5. | SiH ₃ NH ₂ | silanamine (substitutive),
or amidotrihydridosilicon (additive) |
| 6. | PH ₂ Cl | chlorophosphane |
| 7. | PH ₂ Et | ethylphosphane |
| 8. | TIH ₂ OOOTIH ₂ | trioxidanediylbis(thallane) |
| 9. | PbEt ₄ | tetraethylplumbane (substitutive),
or tetraethyllead (additive) |
| 10. | GeH(SMe) ₃ | tris(methylsulfanyl)germane |
| 11. | PhGe(Cl) ₂ (SiCl ₃) | trichloro[dichloro(phenyl)germyl]silane, |

12. MePHSiH₃ not dichloro(phenyl)(trichlorosilyl)germane
methyl(silyl)phosphane,
not (methylphosphanyl)silane or
(silylphosphanyl)methane

For polynuclear parent hydrides, numerical locants are often needed to specify the positions of substituent groups. If there are several equivalent numberings of the parent hydride skeletal atoms relative to the substituents after relevant rules from Section IR-6.2 have been applied, the numbering is chosen which leads to the lowest set of locants for the compound as a whole. If there is still a choice, lowest locants are assigned to the substituent cited first in the name. If no ambiguity arises, some or all locants can be omitted, as in Examples 21 and 22 below. In Ref. 1, preferred names always contain all locants, except if the only locant is the number '1'.

Examples:

13. H₃GeGeGeH₂GeBr₃ 4,4,4-tribromo-2λ²-tetragermane
(numbering of parent fixed by λ designator)
14. $\begin{matrix} & 3 & 2 & & 1 \\ & & & & \\ & & & & \end{matrix}$
H₃SiSiH₂SiH₂COOH trisilane-1-carboxylic acid
15. $\begin{matrix} & 3 & 2 & & 1 \\ & & & & \\ & & & & \end{matrix}$
MeNHN=NH 3-methyltriaz-1-ene (not 1-methyltriaz-3-ene)
(numbering of parent fixed by position of unsaturation)
16. $\begin{matrix} & 1 & & 2 & & 3 & & 4 & & 5 \\ & & & & & & & & & \end{matrix}$
ClSiH₂SiHClSiH₂SiH₂SiH₂Cl
1,2,5-trichloropentasilane (not 1,4,5-)
17. $\begin{matrix} & & & 3 & & 2 & & 1 \\ & & & & & & & \\ & & & & & & & \end{matrix}$
C₃H₇SnH₂SnCl₂SnH₂Br 1-bromo-2,2-dichloro-3-propyltristannane
(1-bromo preferred to 3-bromo)
18. $\begin{matrix} & 1 & & 2 & & 3 & & 4 & & 5 & & 6 & & 7 \\ & & & & & & & & & & & & & \end{matrix}$
HSnCl₂OSnH₂OSnH₂OSnH₂Cl
1,1,7-trichlorotetrastannoxane
- 19.



H-W name: 4-ethyl-2,2-dimethyl-1,3,2,4-diazadisiletane

4-ethyl-2,2-dimethylcyclodisilazane

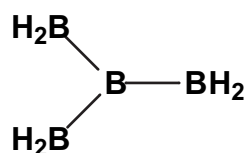
(locant set 2,2,4 preferred to 2,4,4 in both names)

20. $\text{Et}_3\text{PbPbEt}_3$ 1,1,1,2,2,2-hexaethyldiplumbane,
or hexaethyldiplumbane (substitutive),
or bis(triethyllead)(*Pb-Pb*) (additive)
21. MeNHN=Me 1,3-dimethyltriaz-1-ene,
or 1,3-dimethyltriazene

The names of branched structures are based on the longest available unbranched chain, which is regarded as defining the parent hydride, and the names of the shorter chains, which are treated as substituents and appropriately cited. Once the longest chain has been chosen, it is numbered so as to give the lowest set of locants to the substituents.

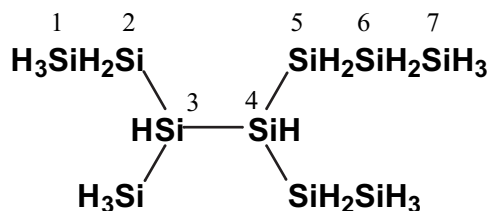
Examples:

22.



2-boranyltriborane(5)

23.



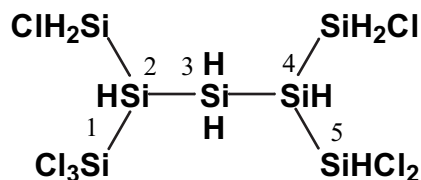
4-disilanyl-3-silylheptasilane

(not 4-disilanyl-5-silylheptasilane)

If a choice of principal chain cannot be made on the basis of chain length alone, unsaturation is the next selection criterion and then the greatest number of substituents.

Example:

24.



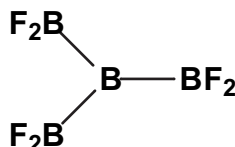
1,1,1,5,5-pentachloro-2,4-bis(chlorosilyl)pentasilane
(all other 5-silicon chains have fewer substituents)

IR-6.3.2 Hydrogen substitution in boron hydrides

The construction of names of derivatives of boron hydrides where hydrogen atoms have been replaced by substituent groups follows the procedures given in Section IR-6.3.1. The only special feature is the need for specifying replacement of a bridging hydrogen atom, in which case the designator ' μ -' is used in front of the substituent group name, as in Example 4 below.

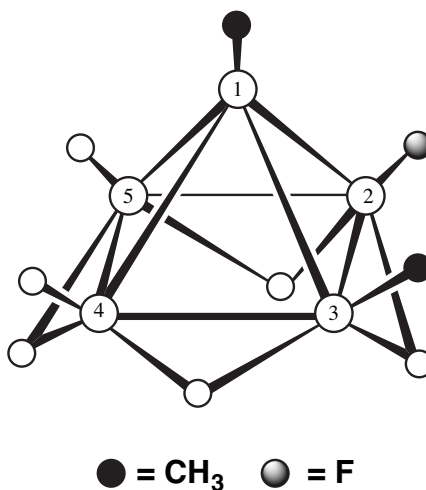
Examples:

1.



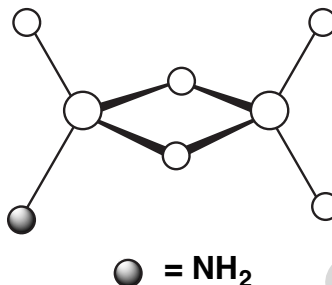
2-(difluoroboranyl)-1,1,3,3-tetrafluorotriborane(5)

2.



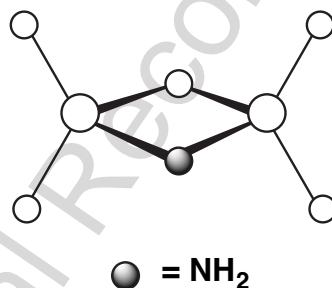
2-fluoro-1,3-dimethylpentaborane(9), or
2-fluoro-1,3-dimethyl-2,3:2,5:3,4:4,5-tetra- μ H-nido-pentaborane(9)

3.



diboran(6)amine

4.

diboran(6)- μ -amine

IR-6.4 NAMES OF IONS AND RADICALS DERIVED FROM PARENT HYDRIDES

This Section presents names of ions and radicals that can be formally derived from hydrides by the operations of removal or addition of hydrogen atoms, hydride ions or hydrons. A great many ions and radicals can also be named by additive methods, as described in Chapter IR-7. Many simple ions and radicals are named in Table IX, often by both nomenclature types.

IR-6.4.1 Cations derived from parent hydrides by addition of one or more hydrons

The name of an ion formally derived by adding a hydron to a parent hydride is obtained by adding the suffix 'ium' to the name of the parent hydride, with elision of a final 'e'. For polycations formed in this way, the suffixes 'dium', 'trium', *etc.*, are used without elision of any final 'e' on the parent hydride name. Any necessary locants are placed immediately preceding the suffix. Locants for added hydrons take precedence over locants for unsaturation, as in Example 8 below.

The alternative names ammonium, diazanium, hydrazinediium and oxonium are used for naming organic derivatives, see Section IR-6.4.3 and Section P-73.1.1 of Ref. 1

Examples:

1. NH_4^+ azanium, or ammonium
2. N_2H_5^+ diazanium, or hydrazinium
3. $\text{N}_2\text{H}_6^{2+}$ diazaniadiium, or hydrazinediium
4. H_3O^+ oxidanium, or oxonium
5. H_4O^{2+} oxidaniadiium
6. H_3O_2^+ dioxidanium
7. H_3PPH_3^+ triphosphane-1,3-diium
8. $^+\text{H}_3\text{N}-\text{N}=\text{NH}$ triaz-2-en-1-ium

IR-6.4.2 Cations derived from parent hydrides by loss of one or more hydride ions

A cation produced by formal loss of a hydride ion from a parent hydride is named by adding the suffix 'ylium' to the parent name, with elision of a final 'e'. (See also, Section P-73.2.2.1 of Ref. 1). For polycations formed in this way, the suffixes 'diylium', 'triylium', *etc.*, are used without elision of any final 'e' on the parent hydride name. Any necessary locants are placed immediately preceding the suffix. Locants for removed hydride ions take precedence over locants for unsaturation, as in Example 5 below.

For the names silane, germane, stannane, plumbane and borane, as well as a number of hydrocarbon names, 'ylium' *replaces* the ending 'ane' of the parent hydride. (See also Section P-73.2.2.1 of Ref. 1).

Examples:

1. PH_2^+ phosphanylium
2. Si_2H_5^+ disilanylium
3. SiH_3^+ silylium
4. BH_2^+ boranylium
5. $^+\text{HN}-\text{N}=\text{NH}$ triaz-2-en-1-ylium

IR-6.4.3 Substituted cations

Names of substituted derivatives of cations are formed from the modified parent hydride names (as described in IR-6.4.1 and IR-6.4.2) by adding appropriate substituent prefixes.

When numbering derivatives of polynuclear parents, the locants for added hydrons or removed hydride ions take precedence over locants for substituents, as in Example 6 below.

Examples:

- | | | |
|----|---|--|
| 1. | [NF ₄] ⁺ | tetrafluoroazanium, or tetrafluoroammonium |
| 2. | [PCl ₄] ⁺ | tetrachlorophosphanium |
| 3. | [NMe ₄] ⁺ | tetramethylazanium, or tetramethylammonium |
| 4. | [SEtMePh] ⁺ | ethyl(methyl)phenylsulfanium |
| 5. | [MeOH ₂] ⁺ | methyloxidanium, or methyloxonium |
| 6. | [ClP ₂ H ₃] ⁺ | 2-chlorodiphosphan-1-ium |

IR-6.4.4 Anions derived from parent hydrides by loss of one or more hydrons

An anion formally obtained by removal of one or more hydrons from a parent hydride is named by adding 'ide', 'diide', *etc.*, to the parent name, with elision of a terminal 'e' before 'ide' but not in any other cases. Any necessary locants are placed immediately preceding the suffix. Locants for removed hydrons take precedence over locants for unsaturation, as in Example 10 below. (See also Section P-72.2.2 of Ref. 1).

Examples:

- | | | |
|-----|---------------------------------|---------------------------|
| 1. | NH ₂ ⁻ | azanide, or amide |
| 2. | HP ²⁻ | phosphanediide |
| 3. | H ₂ NNH ⁻ | diazanide, or hydrazinide |
| 4. | H ₂ NN ²⁻ | diazane-1,1-diide |
| 5. | ⁻ HNNH ⁻ | diazane-1,2-diide |
| 6. | SiH ₃ ⁻ | silanide |
| 7. | GeH ₃ ⁻ | germanide |
| 8. | SnH ₃ ⁻ | stannanide |
| 9. | SH ⁻ | sulfanide |
| 10. | ⁻ HN=N=NH | triaz-2-en-1-ide |

Names of anions derived by formal loss of one or more hydrons from hydroxy groups and their chalcogen analogues (characterized by suffixes such as 'ol' and 'thiol') are formed by adding the ending 'ate' to the appropriate name. (See also, Section P-72.2.2.2 of Ref. 1).

Examples:

- | | | |
|-----|---------------------------------|-------------------|
| 11. | SiH ₃ O ⁻ | silanolate |
| 12. | PH ₂ S ⁻ | phosphanethiolate |

The compound in Example 12 may also be named as a derivative of phosphinothious acid, H_2PSH , thus giving the name 'phosphinothioite'. This type of name is used as the basis for naming organic derivatives of H_2PSH . (See discussion of inorganic acids in Chapter IR-8).

IR-6.4.5 Anions derived from parent hydrides by addition of one or more hydride ions

The addition of a hydride ion to a parent hydride is designated by the ending 'uide' (see Section P-73.2 of Ref. 1). Rules regarding locants are analogous to the rules for the 'ide' suffix (Section IR-6.4.4). For compounds of this kind, additive names (Chapter IR-7) are common and acceptable alternatives.

Example:

1. $[\text{BH}_4]^-$ boranuide (from borane), or tetrahydridoborate(1-) (additive)

IR-6.4.6 Substituted anions

Names of substituted derivatives of anions are formed from parent hydride names modified as above (see Sections IR-6.4.4 and IR-6.4.5) by further adding appropriate prefixes for the substituents. When numbering the structure, the position where a hydron was removed or a hydride ion was added takes precedence over the positions with substituents, as in Example 4 below. In many cases, additive names are common and acceptable alternatives.

Examples:

1. SnCl_3^- trichlorostannanide (from stannane), or trichloridostannate(1-) (additive)
2. CH_3PH^- methylphosphanide
3. CH_3NH^- methylazanide, or methanaminide (see Section P-72.2.2.3 of Ref. 1)
4. $\begin{array}{ccccccc} & 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 \\ \text{Cl}_3\text{SnOSnH}_2\text{OSnH}_2\text{OSnH}_2\text{OSnH}_2^- & & & & & & & & & \end{array}$ 9,9,9-trichloropentastannoxan-1-ide
5. $[\text{BH}_3\text{CN}]^-$ cyanoboranuide (from borane), or cyanidotrihydridoborate(1-) (additive)
6. $[\text{PF}_6]^-$ hexafluoro- λ^5 -phosphanuide (from phosphane), or hexafluoridophosphate(1-) (additive)

IR-6.4.7 Radicals and substituent groups

Radicals and substituent groups derived from parent hydrides by removal of one or more hydrogen atoms are named by modifying the parent hydride name as follows:

- (i) removal of one hydrogen atom: add suffix 'yl' (eliding final 'e' of parent hydride name);
- (ii) removal of two or more hydrogen atoms: add suffix 'yl' with appropriate multiplicative prefix (no vowel elision).

The suffix 'ylidene' is used on a substituent group if a double bond is implied when a skeletal atom has formally lost two hydrogen atoms. If a triple bond is implied, the ending 'ylidyne' is used. With these endings, the ending 'e' of the parent hydride name is again elided.

For radicals, if two hydrogens are removed from the same atom the suffix 'ylidene' is used.

Locants may be needed to indicate the skeletal atoms from which hydrogen atoms have been removed. Such locants are placed immediately before the suffix. When numbering the structure, the positions where hydrogen atoms were removed take precedence over unsaturation, as in Example 10 below.

Radicals may also be named using additive nomenclature, see Section IR-7.1.4.

Examples:

- | | | |
|-----|---|--|
| 1. | NH_2^\bullet | azanylidene |
| 2. | PH_2^\bullet and $\text{H}_2\text{P}-$ | phosphanyl |
| 3. | PH_2^\bullet and $\text{HP}=\text{}$ | phosphanylidene |
| 4. | $\text{HP}<$ | phosphanediyl |
| 5. | $\text{P}\equiv$ | phosphanylidyne |
| 6. | $\text{SiH}_2^{2\bullet}$ | silanylidene |
| 7. | $\text{H}_2\text{Br}^\bullet$ and $\text{H}_2\text{Br}-$ | λ^3 -bromanyl |
| 8. | $\text{NH}_2\text{NH}^\bullet$ and $\text{H}_2\text{NHN}-$ | diazanyl or hydrazinyl |
| 9. | $^\bullet\text{NHNH}^\bullet$ and $-\text{NHNH}-$ | diazane-1,2-diyl or hydrazine-1,2-diyl |
| 10. | $\text{HP}=\text{NP}^\bullet\text{NHPH}^\bullet$ and $\text{HP}=\text{NPNHPH}-$ | triphosphaz-4-ene-1,3-diyl |

In a number of cases, the established name of a substituent group/radical is non-systematic or is a shorter version obtained by *replacing* the ending 'ane' of the parent name by the suffix 'yl':

Examples:

- | | | |
|-----|--|---------------------------------|
| 11. | OH^\bullet | hydroxyl (for oxidanyl) |
| 12. | $\text{OH}-$ | hydroxy (for oxidanyl) |
| 13. | NH_2^\bullet | aminyl (for azanyl) |
| 14. | NH_2- | amino (for azanyl) |
| 15. | $\text{CH}_2^{2\bullet}$ | methylidene (for methanylidene) |
| 16. | SiH_3^\bullet and SiH_3- | silyl (for silanyl) |
| 17. | GeH_3^\bullet and GeH_3- | germyl (for germanyl) |
| 18. | SnH_3^\bullet and SnH_3- | stannyl (for stannanyl) |
| 19. | PbH_3^\bullet and PbH_3- | plumbyl (for plumbanyl) |

This list is exhaustive as far as non-carbon parent hydrides are concerned. A number of established shortened or entirely non-systematic names are also used for carbon-based hydrides: methyl, ethyl, propyl, butyl, pentyl, hexyl, cyclohexyl, phenyl, naphthyl, *etc.*

IR-6.4.8 **Substituted radicals or substituent groups**

Radicals or substituent groups formally derived by removing one or more hydrogen atoms and introducing substituents in parent hydrides are named using prefixes for the substituents as explained in Section IR-6.3.1. The positions from which hydrogen atoms were removed take priority over the positions with substituents. Several simple such radicals and substituent groups are named in Table IX. In a few cases the name of a radical and the corresponding substituent group as used in organic nomenclature may differ (see Example 2 below).

Examples:

- | | | |
|----|--|--|
| 1. | $\text{NH}_2\text{O}^\bullet$ and $\text{NH}_2\text{O}-$ | aminoxidanyl |
| 2. | HONH^\bullet
$\text{HONH}-$ | hydroxyazanyl
hydroxyamine |
| 3. | $\text{Me}_3\text{PbPbMe}_2^\bullet$ and $\text{Me}_3\text{PbPbMe}_2-$ | 1,1,2,2,2-pentamethyldiplumban-1-yl
(not 1,1,1,2,2-pentamethyldiplumban-2-yl) |

IR-6.4.9 **Anionic and cationic centres and radicals in a single molecule or substituent group**

If several of the above features [cationic moiety, anionic moiety, radical formed by removal of hydrogen atom(s)] are present in a molecule or a substituent group, a priority rule is needed to decide in which order to cite the various modifications of the parent hydride name.

The order is:

cation < anion < radical < free valence in substituent group

in the sense that:

- (i) the suffixes indicating these modifications are cited in that order,
- (ii) numbering, if necessary, is started at the position or positions of free valences: in radical species the next lowest locants are given to positions where hydrogen atoms have been removed; then anion sites are numbered; finally cationic sites are numbered. All these take precedence over unsaturation and over substituents cited by prefixes.

Examples:

- | | | |
|----|---|---|
| 1. | $\text{H}_2\text{Te}^{\bullet+}$ | tellaniumyl |
| 2. | $\text{H}_2\text{Te}^{\bullet-}$ | tellanuidyl |
| 3. | $\begin{array}{c} 2 \quad 1 \\ \text{Me}_3\text{N}^+-\text{N}^--\text{Me} \end{array}$ | 1,2,2,2-tetramethyldiazan-2-ium-1-ide |
| 4. | $\begin{array}{c} 3 \quad 2 \quad 1 \\ \text{MeN}=\text{N}^{\bullet+}-\text{N}^--\text{SiMe}_3 \end{array}$ | 3-methyl-1-(trimethylsilyl)triaz-2-en-2-ium-1-id-2-yl |

IR-6.5

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