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INORGANIC CHEMISTRY DIVISION

**COMMISSION ON NOMENCLATURE OF INORGANIC
CHEMISTRY**

**NOMENCLATURE OF INORGANIC
BORON COMPOUNDS**

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**LONDON
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INORGANIC CHEMISTRY DIVISION

COMMISSION ON NOMENCLATURE OF INORGANIC CHEMISTRY†

NOMENCLATURE OF INORGANIC BORON COMPOUNDS

There are certain bonding situations common in boron chemistry and uncommon elsewhere that lead to unusual nomenclature problems.

Excess connectivity or ligancy. In elemental boron each atom has six or seven nearest neighbours. With other elemental non-metals the number of nearest neighbours is four or less and the connections can be assumed to be electron-pair bonds. With boron each atom can contribute only three electrons to its total of six or seven connections. Hence, the connections are not ordinary electron-pair bonds, and structures of many boron compounds cannot be represented by the traditional method of lines for electron pairs. In elemental metals the atoms often have eight to twelve nearest neighbours, but the bonding has no directional character. By contrast, the interatomic bonding in boron is strongly directional. This is accompanied by *clustering by triangles*. Elemental boron may be considered to be composed of close-packed icosahedra of boron atoms with each boron atom connected to five other atoms in the same icosahedron and to one or two atoms in another icosahedron. A regular icosahedron has the highest symmetry of all polyhedra with twenty faces (which in this case are equilateral triangles), twelve vertices (occupied in this case by twelve boron atoms), and thirty edges (or connections between atoms). This icosahedral framework is apparently held together by twenty six electrons, again emphasizing the unusual bonding.

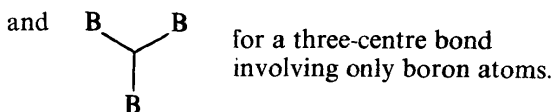
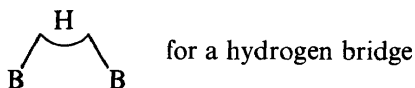
The nomenclature problem is complicated further by the *formation of many molecular hydrides*. Boron forms more known molecular hydrides than any other element except carbon. Many of these have boron skeletons which can be viewed as fragments of an icosahedron. In the neutral hydrides the open edges of the fragments are generally held together by *bridge hydrogen atoms*. In the 'open' boron hydrides there are at the edges of the molecule some hydrogen atoms connected to two boron atoms, a phenomenon largely

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NOMENCLATURE OF INORGANIC BORON COMPOUNDS

unknown in the chemistry of other elements. There are also *unusual fusions*. The icosahedral fragments may be joined by a common vertex, edge or face, leading to even higher connectivities at the joining atoms and further unprecedented nomenclature problems.

It is possible to explain the bonding in all the above cases as being due to localized *three-centre bonds*, i.e. a pair of electrons being shared among three atoms. Hence, it is convenient to have a conventional representation for a three-centre bond, just as a line is used for the two-centre bond. The representations commonly used are



However, for elemental boron and for all but the two simplest boron hydrides, several equally valid three-centre bonding representations can be drawn. Hence, just as the normal localized bond representation for benzene is inadequate, representation of the bonding by using localized three-centre bonds is inadequate in all but the simplest boron compounds.

For nomenclature of these volatile boron hydrides nearly all the precedents and suggestions have been based on alkane and silane chemistry. However, the bonding and structures are quite different.

Parent hydrides with negative charge. In many stable boron-containing entities, the entity has extra electrons beyond those that it and other bonded atoms can contribute: e.g. in $[\text{BH}_4]^-$, isoelectronic with methane, and in $[\text{B}_{12}\text{H}_{12}]^{2-}$ which contains the icosahedron referred to above. The last entity has more possible derivatives than benzene. Present nomenclature schemes do not conveniently handle the known range of substitution derivatives of such an anion. Substitution for hydrogen by positive radicals (or experimentally, substitution of hydride ions by neutral molecules) leads to neutral and cationic species that may be logically viewed as derivatives of anions, e.g. $[\text{B}_{12}\text{H}_9(\text{NH}_3)_3]^{1+}$. Also replacement of boron atoms by other non-metal atoms (stripped to three valence electrons to be isoelectronic with boron) leads to neutral and cationic replacement derivatives of the boron hydride anions: e.g. $\text{B}_{10}\text{C}_2\text{H}_{12}$, $\text{B}_{11}\text{PH}_{12}$ and $[\text{B}_{11}\text{SH}_{12}]^+$. All these examples have skeletons isoelectronic with $[\text{B}_{12}\text{H}_{12}]^{2-}$. Such skeletons are conveniently named by postulating *unknown parent species* (see **Rules 2.3** and **7**.) In the nomenclature of other elements this rarely occurs, e.g. orthocarbonic acid, but in the chemistry of boron it is commonplace. Since the parent entities are anions, another set of nomenclature precedents comes from inorganic coordination nomenclature.

*Index to rules**Rule No. Subject*

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7. Boranes with skeletal replacement
8. Addition compounds

RULES**Rule 1. General**

The root of the word boron is 'bor-' and this is used to designate the presence of boron. This root leads to the following applications:

in replacement nomenclature	bora-
presence of both boron and hydrogen	boran-
boron anion	borate

1.1 Binary boron compounds may be named according to stoichiometric nomenclature^{1a}.

Examples:

1. BCl_3 boron trichloride
2. B_2F_4 diboron tetrafluoride
3. B_2O_3 diboron trioxide
4. TiB_2 titanium diboride
5. AlB_{12} aluminium dodecaboride
6. B_{12}C_3 dodecaboron tricarbide
7. CaB_6 calcium hexaboride

However, for more complex substances the following rules are needed.

Rule 2. Boron hydrides

2.1 Boron hydrides are called *boranes* and the name of BH_3 is *borane*. The name borine should be abandoned.

2.2 The number of boron atoms in the molecule is indicated by an appropriate numerical prefix. (The Latin nona and undeca are used instead of the Greek ennea and hendeca to conform with hydrocarbon nomenclature. It is recommended that the prefix for twenty be spelled icoso rather than eicosa to agree with common practice in geometry as opposed to the practice in organic hydrocarbon nomenclature.)

2.3 The number of hydrogen atoms in the molecule is indicated by enclosing the appropriate Arabic numeral in parentheses directly following the name.

Examples:

1. BH_3 borane(3)
2. B_2H_6 diborane(6) (*Figure 1*)
3. B_3H_7 triborane(7)
4. B_4H_{10} tetraborane(10) (*Figure 2*)
5. B_5H_9 pentaborane(9) (*Figure 3*)
6. B_5H_{11} pentaborane(11) (*Figure 4*)

7. B_6H_{10} hexaborane(10) (Figure 5)
8. $B_{10}H_{14}$ decaborane(14) (Figure 9)
9. $B_{10}H_{16}$ decaborane(16) (Figure 10)
10. $B_{20}H_{16}$ icosaborane(16) (Figure 18)

At present examples 1 and 3 are un-isolated parent species (see **Rules 3 and 8**).

These names are based on molecular formulae rather than structures. Unambiguous definition of structure would lead to extremely complex names (see figures).

In practice, it is permissible to drop the numerical designation of the number of hydrogen atoms in borane(3) and in other cases where no ambiguity results, but this must be done judiciously.

Examples :

1. BH_3 borane
2. B_2H_6 diborane

During the period when the differences in the structures of two or more isomers were not known such prefixes as iso and neo have been used to distinguish isomers. Once structures are known, a structural name is preferred (see **Rule 2.31**).

2.31 Boranes that may be considered to be formed by fusion or joining of simpler boranes with loss of hydrogen may also be named as derivatives of the simpler boranes. (For numbering practices see **Rule 3.22** and **3.25**.)

Examples :

1. $B_{10}H_{16}$ 1,1'-bipentaboran(9)yl or 1,1'-bipentaborane(9)^{2a} (Figure 10)
See example (1) section **4.22** for the radical name
2. $B_{18}H_{22}$ decaborano(14)[6',7':5,6]decaborane(14) (Figure 19)
3. iso- $B_{18}H_{22}$ decaborano(14)[6',7':6,7]decaborane(14) (Figure 19)

Examples 2 and 3 are fusion type names formed in the same manner as for organic compounds, e.g. benzofuran^{2b}.

2.4 The polyboranes and their derivatives are of two general classes: (1) closed structures (that is, structures with boron skeletons that are polyhedra having only triangular faces) and (2) non-closed structures. The members of the first class are designated by the italicized prefix *closo*. Some members of the second class have structures very close to a closed structure. When it is desirable to indicate this situation in contrast to a known *closo*-compound, the italicized prefix *nido* from the Latin *nidus* for nest is used.

Examples :

1. B_4Cl_4 tetrachloro-*closo*-tetraborane(4)
2. $B_{10}H_{14}$ *nido*-decaborane(14) (Figure 9)
3. $B_{20}H_{16}$ *closo*-icosaborane(16) (Figure 18)

The need for these prefixes becomes more evident in naming heteroboranes and boron hydride anions (see **Rules 5.4** and **7**).

Rule 3. Derivatives of the boranes

3.1 Derivatives of borane, BH_3 , are named by substitution rules^{2c} as in the following examples.

Examples :

1. BCl_2H dichloroborane
2. BH_2SbH_2 stibinoborane
3. BBr_2F dibromofluoroborane
4. BCl_2I dichloriodoborane
5. $\text{B}(\text{OH})_3$ trihydroxyborane
6. $\text{BCH}_3(\text{OH})_2$ dihydroxymethylborane
7. $\text{B}(\text{CH}_3)_2\text{OH}$ hydroxydimethylborane
8. $\text{BCl}(\text{OCH}_3)_2$ chlorodimethoxyborane

$\text{B}(\text{OH})_3$ may also be called orthoboric acid^{1b}. Borinic and boronic acid names are not approved.

The substituents are listed alphabetically. Borane takes precedence as the root name over elements in main groups IV to VII inclusive. This is in harmony with the practice for organometallic and metal-metal bonded compounds^{1c}.

3.2 Derivatives of the polyboranes formed by substitution of an atom or group for hydrogen are named as substitution derivatives according to standard organic practices^{2a, b}.

3.21 When a polyborane is fully substituted by the same substituent or when only the number and not the position of substituent groups is known, only the number of substituent groups is designated. The numerical suffix of the parent must be retained in substituted polyboranes.

Examples :

1. B_2Br_4 tetrabromodiborane(4)†
2. B_8Cl_8 octachlorooctaborane(8)†
3. $\text{B}_2\text{H}_5\text{Cl}$ chlorodiborane(6)
4. $\text{B}_{10}\text{H}_4\text{I}_{10}$ decaiodododecaborane(14)

3.22 Numbering practices

In general the use of symbols and numbers follows standard practices of organic nomenclature^{2a, b}. Additional practices are introduced in **Rule 2.3** and below.

3.221 Numbering of positions in open boron frameworks

For numbering purposes the open boron frameworks are viewed as plane projections from opposite the open portion of the framework. The boron atoms are numbered by zones with the interior atoms of the projection being numbered first followed by the peripheral atoms. Each zone of atoms is numbered clockwise (e.g. B_5H_9 *Figure 3*). In more complex cases numbering in each zone is started at an arbitrary twelve o'clock position selected by as many as necessary of the following criteria taken in order:

(a) The molecule is oriented so that the twelve o'clock position lies in a symmetry plane containing as few atoms as possible (e.g. see *Figure 1* for diborane, *Figure 2* for B_4H_{10} and *Figure 3* for B_5H_9).

(b) The molecule is oriented so that the twelve o'clock position will be in the portion of this symmetry plane containing the greater number of atoms (e.g. B_5H_{11} *Figure 4*, B_6H_{10} *Figure 5*, $\text{B}_9\text{H}_{13}\text{L}$ *Figure 8*, $\text{B}_{11}\text{H}_{13}\text{L}$ *Figure 11*).

† Compare **Rule 1.1** for stoichiometric name, e.g. example 2.

(c) The molecule is oriented so that the twelve o'clock position lies opposite the greater number of bridge hydrogens (e.g. B_8H_{12} *Figure 6*, B_9H_{15} *Figure 7*).

For boranes with skeletal replacement, the numbering is based on a parent *boron skeleton* with all boron–boron bonds equivalent. Lowest numbering for hetero atoms takes priority over (c). See **Rule 7.4** example 2.

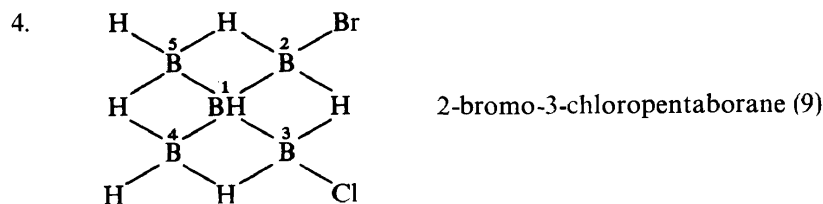
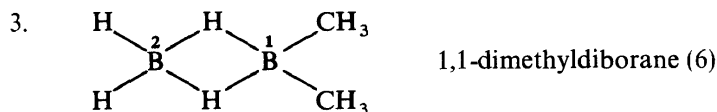
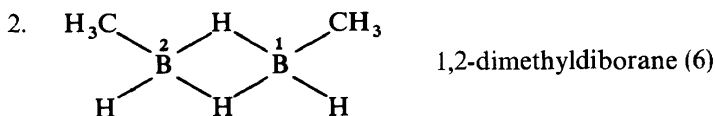
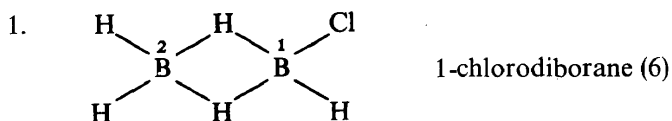
Boron frameworks which lack only one atom to complete a regular polyhedron are numbered by **Rule 3.25** for closed frameworks. Missing boron atoms should normally be numbered last and, if necessary, designated by 'debor'. This generally gives numberings in agreement with the preceding rules. See **Rule 7.5** examples 3 and 4.

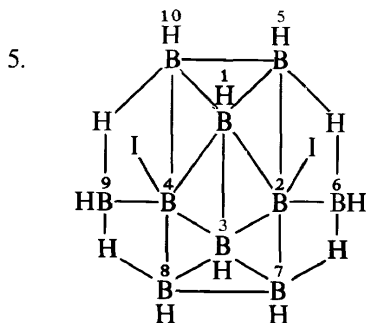
This system gives different numberings for stereoisomers. For optical enantiomers whose absolute configurations are unknown, the name should use lowest numbering and be preceded by an italic *X*. This practice is in agreement with the rules for coordination compounds^{1d}.

3.222 Naming non-bridging substituents

The appropriate prefix is directly attached to the name of the parent compound and is numbered corresponding to the boron atom to which the substituent is attached, the number being as low as possible.

Examples :





2,4-diiodododecaborane (14)
(cf. Figure 9)

It should be understood that the lines above do not imply conventional covalent bonds, but only close 'connections'.

3.23 Presently known boron hydrides containing BH_2 groups may be considered fragments of an icosahedron. In such structures one hydrogen of the BH_2 group is directed away from the centre of the parent icosahedron whereas the second hydrogen is directed in a general fashion along the missing surface. Substitution at the former type of hydrogen is designated by the italicized prefix *exo* and at the latter by the italicized prefix *endo*.

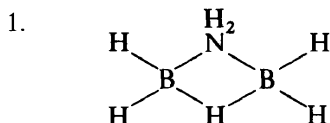
Example:

$(\text{CH}_3\text{CN})_2\text{B}_{10}\text{H}_{12}$ is an *exo* compound (see Figure 12)

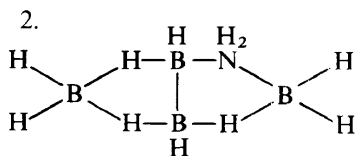
3.24 Substituents for hydrogen atoms in bridge positions are designated by use of the symbol ' μ ' as a prefix to the name of the substituent^{1c}.

If it is necessary to distinguish between bridge positions, the bridge positions are indicated by designating the numbers of the boron atoms across which bridging occurs followed by a hyphen. The lowest possible numbers are used to designate points of bridging as is done for substituents.

Examples:



μ -aminodiborane (6)



1,2- μ -aminotetraborane (10)

Note that hydrogen bridges are not specifically designated.

3.25 Numbering of closed boron frameworks. For use of *closo*, see **Rule 2.4**.

The boron atoms are numbered in sequential planes perpendicular to the longest highest-order symmetry axis. The atoms in each plane are numbered clockwise from a reference symmence plane through this symmetry axis. For cases where the orientation is critical, the molecule is viewed down this axis as a planar projection and oriented by the sequential criteria of **3.221** (e.g. see Figure 17).

This is in harmony with the rules for coordination polyhedra^{1f}.

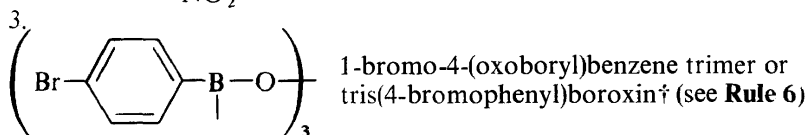
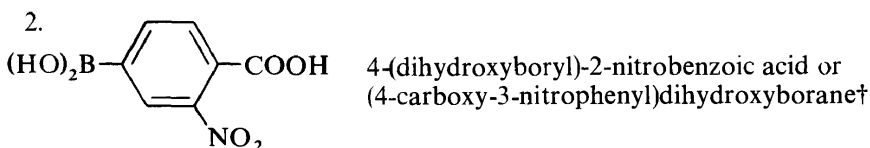
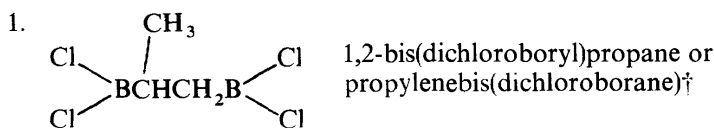
Rule 4. Boron radicals

4.1 Radicals derived from borane, BH_3 , are named by replacing the suffix 'ane' by 'yl' or by using the root 'borio' from *Table V* of ref. 1 for the linking atom and naming the ligands attached to boron:

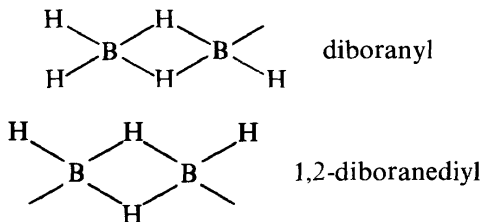
$\text{H}_2\text{B}-$	boryl or dihydroborio
$\text{Cl}_2\text{B}-$	dichloroboryl or dichloroborio
$(\text{CH}_3)_2\text{B}-$	dimethylboryl or dimethylborio
$(\text{HO})_2\text{B}-$	dihydroxyboryl or dihydroxoborio
$\text{OB}-$	oxoboryl or oxoborio
$\text{HB}<$	boranediyl or hydroborio
$\text{CH}_3\text{B}<$	methylboranediyl or methylborio
$\text{HOB}<$	hydroxyboranediyl or hydroxoborio
$\text{B}<<$	boranetriyl or borio

Polyboranyl is used here for polyboron radicals to avoid confusion with multiple $-\text{BH}_2$ groups. Thus, diboryl means two $-\text{BH}_2$ groups and diboranyl is the monovalent radical derived from diborane.

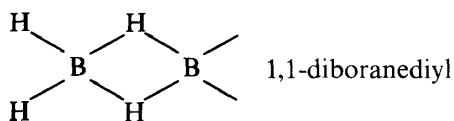
Examples:



4.2 Radicals derived by removal of terminal hydrogen atoms from boron hydrides containing two or more boron atoms are named as follows:

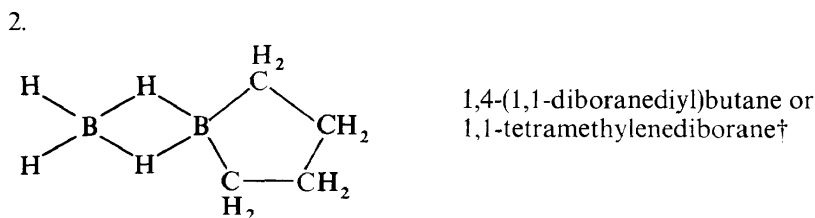
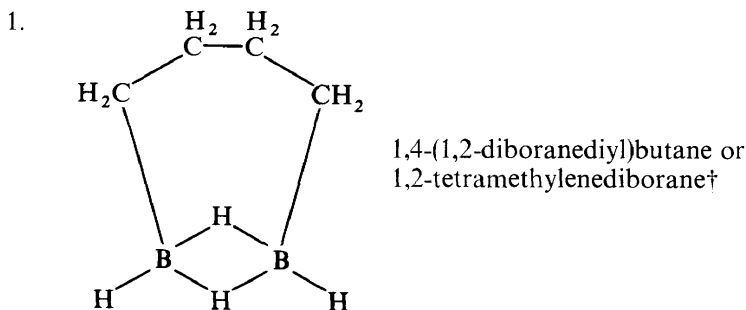


[†] Preferred name—see **Rule 3.1**.



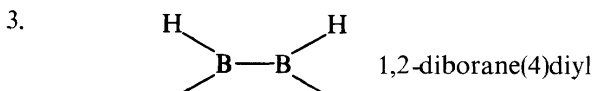
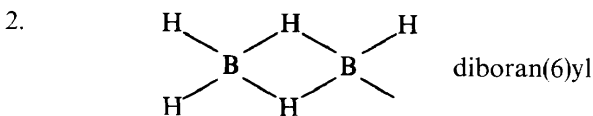
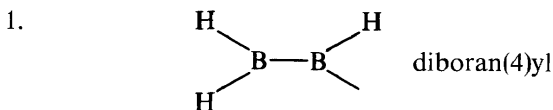
—(B₁₀H₁₂)— 6,9-decaborane (see Figure 9)

Examples:



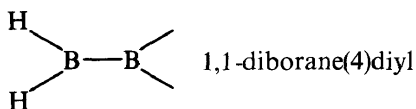
4.21 Radicals derived from several boron hydrides containing the same number of boron atoms but different numbers of hydrogen atoms may be distinguished by retaining in parentheses the Arabic numeral indicating the number of hydrogen atoms in the parent borane after the syllable ‘-an’ and before the radical ending.

Examples:



† Preferred name—see Rule 3.1.

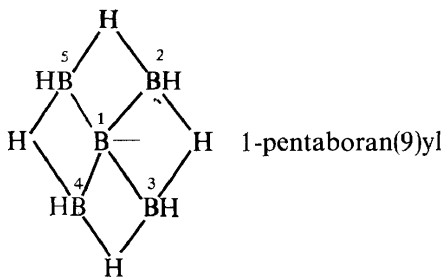
4.



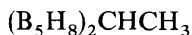
4.22 The position of attachment of a radical shall be given the lowest possible locant and is indicated by placing the appropriate numeral or symbol before the radical name.

Examples:

1.

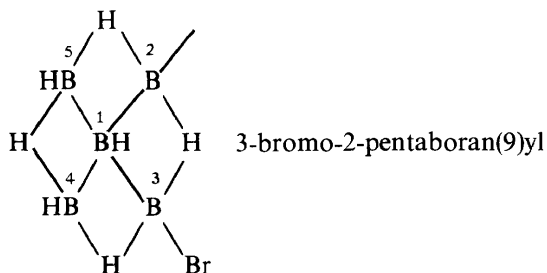


2.



1,1-bis[1-pentaboran(9)yl]ethane or
1,1'-ethylidenebis[pentaborane(9)]†

3.

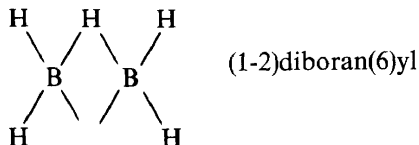


4.3 Radicals formed by removal of bridging hydrogen atoms

These are named as in **Rule 4.2** and attachment at the bridging position is indicated by listing the atoms to which the bridge is attached, separated by a hyphen and enclosed in parentheses.

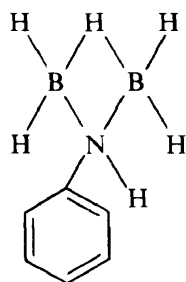
Examples:

1.



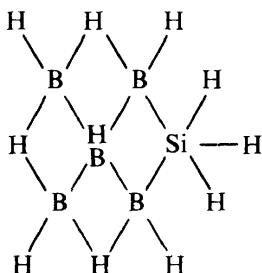
† Preferred name—see **Rule 3.1**.

2.



N-(1-2)diboranylamine or
 μ -anilinodiborane(6)[†]

3.



(2-3)pentaboran(9)ylsilane or
 μ -silylpentaborane(9)[†]

Rule 5. Ions related to boron hydrides

5.1 Boron-containing ions and their salts may be named according to the rules for naming coordination compounds^{1g}.

Examples:

- | | |
|--|--|
| 1. NaBF ₄ | sodium tetrafluoroborate |
| 2. LiBH ₄ | lithium tetrahydroborate |
| 3. Th(BH ₄) ₃ | thorium tris(tetrahydroborate) or
thorium(III) tetrahydroborate |
| 4. NH ₄ [B(C ₆ H ₅) ₄] | ammonium tetraphenylborate |
| 5. [(CH ₃) ₄ N][BCl ₄] | tetramethylammonium tetrachloroborate |

The prefix 'tetra-' may be dropped if no ambiguity results.

Examples:

- | | |
|----------------------|---------------------|
| 6. NaBF ₄ | sodium fluoroborate |
| 7. LiBH ₄ | lithium hydroborate |

'Pseudo binary names' such as borofluoride and borohydride should be abandoned.

5.2 To indicate the charge of the ion the Ewens-Bassett system^{1h} is used. The Stock system^{1h} is not recommended because in the polyboron ions the oxidation numbers are generally non-integral (see following rules).

Examples:

- | | |
|--|---|
| 1. Na[BH ₃ CN] | sodium cyanotrihydroborate(1-) |
| 2. Ca[B(CH ₃) ₂ H] | calcium hydrodimethylborate(2-) |
| 3. [BH ₂ (NH ₃) ₂]Cl | diamminedihydroboron(1+) chloride |
| 4. [Re(H ₃ B) ₂ (CO) ₅] ⁻ | bis(borane)pentacarbonylrhenate(1-) ion |

[†] Preferred name—see Rule 3.1.

- | | |
|--|---|
| 5. Ba [BF ₂ (OH) ₂] ₂ | barium difluorodihydroxoborate(1 -) |
| 6. K ₂ [Zn ₃ (BH ₄) ₈] | potassium octakis(tetrahydroborato)trizincate-(2 -) |
| 7. Na ₂ [H ₃ BCO ₂] | sodium carboxylatotrihydroborate(2 -) |
| 8. Na [BH ₃ CONH ₂] | sodium carbamoyltrihydroborate(1 -) |

The prefix borano has been used for the BH₃ group as a replacement for oxygen in the naming of some anions, but is not recommended; e.g. the anions of examples 7 and 8 have been called boranocarbonate and boranocarbamate.

5.3 Ionic polyboron compounds may be named by simple extension of the pattern for mononuclear compounds. Ionic polyboron oxygen compounds (polyborates) may be named similarly or by the rules for naming isopolyanions¹¹. Neutral derivatives may be named by this system or by addition nomenclature (see **Rule 8**).

Examples:

- | | |
|--|--|
| 1. Na [B ₂ H ₇] | sodium heptahydrodiborate(1 -) |
| 2. Na ₂ [B ₂ (C ₆ H ₅) ₆] | sodium hexaphenyldiborate(2 -) |
| 3. Ca [B ₃ H ₈] ₂ | calcium octahydrotriborate(1 -) |
| 4. Na [B ₉ H ₁₄] | sodium tetradecahydro-nonaborate(1 -) |
| 5. Na ₂ [B ₁₀ Cl ₁₀] | sodium decachlorodecaborate(2 -) |
| 6. Na ₂ [B ₁₀ H ₁₀] | sodium decahydrodecaborate(2 -) |
| 7. Na [B ₁₀ H ₉ NH ₃] | sodium amminenonahydrodecaborate(1 -) |
| 8. B ₁₀ H ₈ (NH ₃) ₂ | diammineoctahydrodecaboron |
| 9. [B ₁₀ H ₇ (NH ₃) ₃] ⁺ | triammineheptahydrodecaboron(1 +) ion |
| 10. [B ₁₀ H ₈ (COOH) ₂] ²⁻ | dicarboxy-octahydrodecaborate(2 -) ion |
| 11. Na ₂ B ₄ O ₇ | sodium hepta-oxotetrate(2 -) or sodium tetraborate ¹¹ |

5.4 Prefixes, such as *nido* and *closo* for open and closed boron frameworks respectively, may be used when required for clarity, as in **Rule 2.4**.

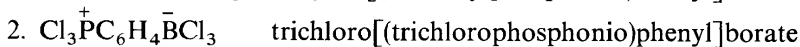
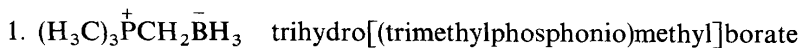
Examples:

- | | |
|--|---|
| 1. Na ₂ [B ₁₀ H ₁₀] | sodium decahydro- <i>closo</i> -decaborate(2 -) |
| 2. Na ₂ [B ₁₀ H ₁₂] | sodium dodecahydro- <i>nido</i> -decaborate(2 -) |
| 3. Na [B ₁₀ H ₁₃] | sodium tridecahydro- <i>nido</i> -decaborate(1 -) |
| 4. Na ₂ [B ₁₀ H ₁₄] | sodium tetradecahydro- <i>nido</i> -decaborate(2 -) |
| 5. Na [B ₁₀ H ₁₅] | sodium pentadecahydro- <i>nido</i> -decaborate(1 -) |
| 6. [B ₁₂ H ₁₂] ²⁻ | dodecahydro- <i>closo</i> -dodecaborate(2 -) ion |
| 7. [B ₁₂ H ₁₁ Cl] ²⁻ | chloroundeca-hydro- <i>closo</i> -dodecaborate(2 -) ion |
| 8. [B ₁₂ H ₁₁ NH ₃] ⁻ | amineundeca-hydro- <i>closo</i> -dodecaborate(1 -) ion |
| 9. B ₁₂ H ₁₀ (NH ₃) ₂ | diamminedeca-hydro- <i>closo</i> -dodecaboron |

The term boranate has been used to describe boron hydride anions. Attempts to generalize such a system to include cations result in conflicts with inorganic coordination nomenclature rules concerning suffixes. Hence, in the interest of uniformity with other inorganic nomenclature, such a system is not recommended.

5.5 Dipolar ions. The presence of boron and atoms of groups V and VI of the Periodic Table in the same molecule gives rise to the possibility of large numbers of dipolar ion molecules. These are best named as substituted borate anions.

Examples:



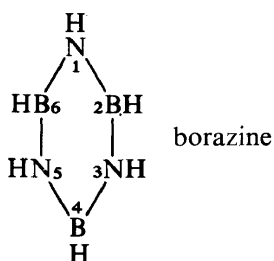
Addition type names such as trimethylphosphinemethylene-borane for example (1) are not recommended.

Rule 6. Inorganic boron heterocyclic compounds

6.1 There are a few inorganic ring systems containing boron that are particularly stable and consequently give rise to a considerable number of derivatives. Such rings usually arise from alternate boron atoms and atoms of group V or VI elements. Accepted trivial names follow:

Example:

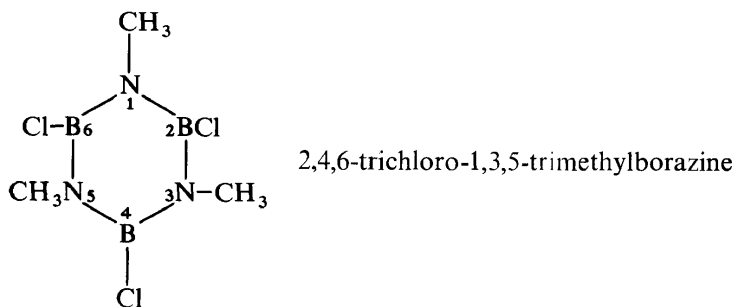
1.



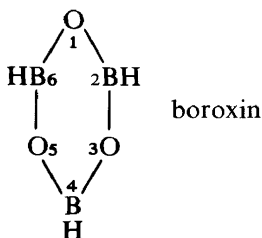
The order of numbering of the ring atoms follows organic heterocyclic nomenclature^{2d}.

Examples:

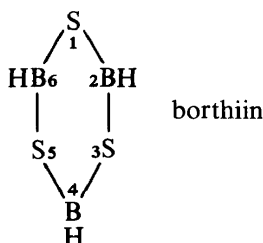
1.



2.



3.

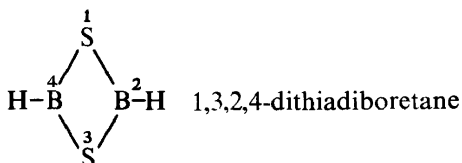


The names borazole, boroxole and borthiole imply five-membered rings and should be abandoned.

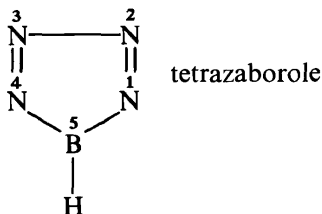
6.2 The following rings and other small rings of atoms with 'normal' valencies may be named by the Hantzsch–Widman system as described in ref. 2, **Rule B-1** (especially *Tables I and II*).

Examples:

1.



2.



One of the most difficult problems in inorganic nomenclature involves description of rings and chains with elements having 'unusual' coordination numbers, e.g. $(\bar{\text{B}}\text{H}_2^+\bar{\text{N}}\text{H}_2)_3$, $(\bar{\text{B}}\text{H}_2^+\bar{\text{P}}\text{H}_2)_4$, and $(\bar{\text{P}}\text{X}_2^+\bar{\text{N}})_4$. At present, these compounds are probably best named as oligomers of the monomeric species having ordinary coordination numbers, i.e. the first example is aminoborane cyclic trimer and the second is phosphinoborane cyclic tetramer.

Rule 7. Boranes with skeletal replacement

7.1 The names of the general classes of compounds in which one or more boron atoms in a network have been replaced by a hetero atom are formed by an adaptation of organic replacement nomenclature^{2f} as carbaboranes, azaboranes, phosphaboranes, thiaboranes, etc.

In this adaptation, a boron atom is replaced by the replacing atom irrespective of valence. For example, $\text{B}_{10}\text{C}_2\text{H}_{12}$ is very stable, has many known derivatives, and is named dicarbadodecaborane, as the dicarba replacement derivative of the unknown $\text{B}_{12}\text{H}_{12}$. It is isoelectronic with and is in this respect a replacement derivative of the very stable $[\text{B}_{12}\text{H}_{12}]^{2-}$ anion.

In organic replacement nomenclature a methylene (CH_2) group is re-

placed variably by an E, EH or EH_2 group where E is the replacing hetero element. This practice is possible because of the stable bonding capacity of carbon which leads to a calculable number of hydrogen atoms from a name based on the number of carbons and the number and type of multiple bonds. A stable bonding capability is also assumed for the replacing hetero element. e.g. sulfur, boron, and silicon are assumed to form only two, three and four bonds, respectively^{2e}. In boron compounds, however, the number of hydrogens bears no simple relationship to the number of boron atoms and must be indicated by a numerical suffix (see **Rule 2.3**). In the hetero polyboranes the number of nearest neighbours for both the boron and hetero atoms is generally five or six (see also the introduction to these rules). Thus, in the adaptation of organic replacement nomenclature to polyboron compounds, the replacement of boron by another atom is indicated along with the total number of hydrogens in the replacement compound.

The prefixes *closo* and *nido* indicate closed and open networks as in **Rule 2.4**. The positions of the hetero atoms in the cage or network are indicated by the lowest possible numbers consistent with the numbering of the parent polyborane (see **Rules 3.221** and **3.25**). Since the number of bridge hydrogens in *nido* heteroboranes is different from that in the parent polyboranes, only the symmetry of the boron skeleton of the parent polyborane is considered in numbering. For this purpose all boron–boron bond lengths are to be considered equivalent.

Examples:

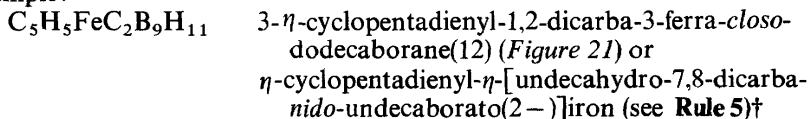
- | | | |
|--|---|-----------|
| 1. $\text{B}_3\text{C}_2\text{H}_5$ | dicarba- <i>closo</i> -pentaborane(5) | |
| 2. $\text{B}_4\text{C}_2\text{H}_6$ | 1,2-dicarba- <i>closo</i> -hexaborane(6) | |
| 3. $\text{B}_4\text{C}_2\text{H}_6$ | 1,6-dicarba- <i>closo</i> -hexaborane(6) | |
| 4. B_5CH_7 | carba- <i>closo</i> -hexaborane(7) | |
| 5. $\text{B}_4\text{C}_2\text{H}_8$ | 2,3-dicarba- <i>nido</i> -hexaborane(8) | |
| | (for numbering see <i>Figure 5</i>) | |
| 6. $\text{B}_3\text{C}_3\text{H}_7$ | 1,2,3-tricarba- <i>nido</i> -hexaborane(7) | |
| | (for numbering see <i>Figure 5</i>) | |
| 7. $\text{B}_5\text{C}_2\text{H}_7$ | dicarba- <i>closo</i> -heptaborane(7) | |
| 8. $\text{B}_6\text{C}_2\text{H}_8$ | dicarba- <i>closo</i> -octaborane(8) | |
| 9. $\text{B}_8\text{C}_2\text{H}_{10}$ | dicarba- <i>closo</i> -decaborane(10) | |
| 10. $\text{B}_9\text{C}_2\text{H}_{13}$ | 7,8-dicarba- <i>nido</i> -undecaborane(13) | |
| | (for numbering see <i>Figure 11</i>) | |
| 11. $\text{B}_{10}\text{C}_2\text{H}_{12}$ | 1,2-dicarba- <i>closo</i> -dodecaborane(12) | } isomers |
| | 1,7-dicarba- <i>closo</i> -dodecaborane(12) | |
| | 1,12-dicarba- <i>closo</i> -dodecaborane(12) | |
| | (for numbering see <i>Figure 16</i>) | |
| 12. $\text{B}_{11}\text{PH}_{12}$ | phospha- <i>closo</i> -dodecaborane(12) | |
| | (for numbering see <i>Figure 16</i>) | |
| 13. $\text{B}_{10}\text{CPH}_{11}$ | 1-phospha-2-carba- <i>closo</i> -dodecaborane(11) | |
| | (for numbering see <i>Figure 16</i>) | |
| 14. $\text{B}_{10}\text{SH}_{12}$ | 7-thia- <i>nido</i> -undecaborane(12) | |
| | (for numbering see <i>Figure 11</i>) | |

Carborane has been used both as a class name for the carbaboranes and also as a trivial name for $\text{B}_{10}\text{C}_2\text{H}_{12}$ and the isomers have been called *ortho*, *meta*

and *para*. Barene has also been used as a trivial name for $B_{10}C_2H_{12}$. These names are not recommended.

7.2 When a *closo* structure is completed by a metal atom, numbering is simplified by considering the metal atom to be part of the cage. Such structures may be named by the principles of replacement nomenclature given above. Alternatively, they may be named as a *nido* ligand bonded to the metal atom†.

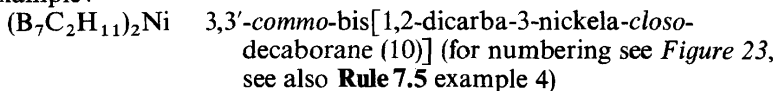
Example:



The trivial name dicarbollyl has been used for the ligand $B_9C_2H_{11}^{2-}$. However, this system is not extensible to other ligands which behave similarly, such as $B_7C_2H_{11}^{2-}$, and therefore its use is not recommended.

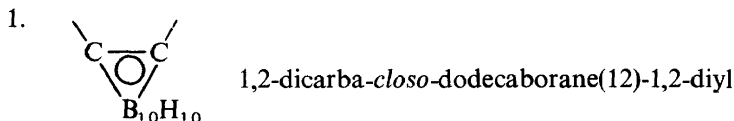
7.3 When a metal atom is shared between two borane cages the prefix *commo* is suggested.

Example:

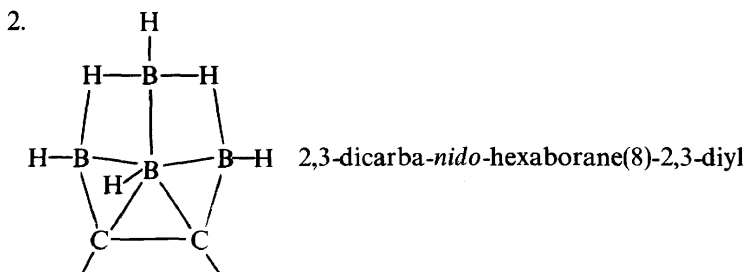


7.4 Radicals derived from heteroboranes are named by following the system described in **Rule 4**.

Examples:



The circle in this formula indicates a delocalized electronic system³.



† Practice in this case is in agreement with ref. 1j.

7.5 Ions derived from heteroboranes are named by the principles of **Rule 5**.

Examples :

- $$\left[\begin{array}{c} \text{HC} \quad \text{CH} \\ \diagdown \quad \diagup \\ \text{O} \\ \diagup \quad \diagdown \\ \text{B}_{10}\text{H}_{10} \end{array} \right]^{2-}$$
 dodecahydro-1,2-dicarba-*nido*-dodecaborate(2-)
- $$\left[\begin{array}{c} \text{C} \quad \text{C} \\ \diagdown \quad \diagup \\ \text{O} \\ \diagup \quad \diagdown \\ \text{B}_{10}\text{H}_{10} \end{array} \right]^{2-}$$
 (*B*-decahydro)-1,2-dicarba-*closo*-dodecaborate(2-)
- $$[\text{B}_9\text{C}_2\text{H}_{11}]^{2-}$$
 undeca-hydro-7,8-dicarba-*nido*-undecaborate(2-) or undeca-hydro-7,8-dicarba-12-debor-*closo*-dodecaborate(2-) (for numbering see *Figure 11*)
- $$[(\text{B}_7\text{C}_2\text{H}_9)_2\text{Fe}]^{1-}$$
 bis [η -nona-hydro-5,9-dicarba-*nido*-nonaborato]ferrate(1-) or bis [η -nona-hydro-1,2-dicarba-3-debor-*closo*-dodecaborato]ferrate(1-) (see *Figure 23* for structure and another type name using **Rule 7.3**)

Rule 8. Addition compounds

A large number of boron-containing compounds may be prepared from or considered formally as the union of an electron pair donor compound with a boron compound. Hence they are named as addition compounds even though some of them are not formed in this simple fashion. The boron-containing compound which functions as the acceptor is named last but followed by water if present.

8.1 The donor molecule and boron compound are each given their proper names with the donor first, and joined by a dash.

8.2 The number of hydrogens in the borane or polyborane parent structure (known or postulated) is given the appropriate Arabic numeral in the customary manner.

Examples :

- $(\text{CH}_3)_3\text{N} \cdot \text{BH}_3$ trimethylamine-borane
- $(\text{CH}_3)_3\text{N} \cdot \text{B}_3\text{H}_7$ trimethylamine-triborane(7)
- $2\text{CH}_3\text{CN} \cdot \text{B}_{10}\text{H}_{12}$ *exo*-6,9-bis(acetonitrile)-decaborane(12) (*Figure 12*)
- $2\text{NH}_3 \cdot \text{B}_{12}\text{H}_{10}$ diammonia-dodecaborane(10)
- $2\text{C}_2\text{H}_5\text{NH}_2 \cdot \text{B}_5\text{H}_9$ bis(ethylamine)-pentaborane(9)
- $2\text{N}_2 \cdot \text{B}_{12}\text{H}_{10}$ bis(dinitrogen)-dodecaborane(10)
- $2(\text{CH}_3)_2\text{S} \cdot \text{B}_{10}\text{Cl}_6\text{H}_2$ bis(dimethyl-sulfide)-hexachloro-decaborane(8)
- $\text{BF}_3 \cdot 2\text{H}_2\text{O}$ boron fluoride-dihydrate
- $\text{Na}_2\text{B}_4\text{O}_7 \cdot 10\text{H}_2\text{O}$ disodium tetraborate-decahydrate

8.3 If there are possible alternatives in the manner of attachment of the ligand to the boron or when it is desired to emphasize the manner of attach-

ment, the dash is replaced by parentheses enclosing the symbols of the two elements forming the bond separated by a dash.

Examples:

1. $\text{OC} \cdot \text{BH}_3$
2. $(\text{CH}_3)_3\text{N} \cdot \text{BH}_2\text{NH}_2$
3. $\text{BH}_2\text{NH}_2 \cdot \text{BF}_3$
4. $(\text{CH}_3)_3\text{N} \cdot \text{BHCH}_3\text{NHCH}_3$
5. $\text{CH}_3\text{ONH}_2 \cdot \text{BH}_3$
6. $(\text{C}_5\text{H}_5)_2\text{H}_2\text{W} \cdot \text{BF}_3$
7. $\text{CH}_3\text{NH}_2 \cdot \text{B}_{10}\text{CH}_{12}$

carbon monoxide (*C-B*)borane
 trimethylamine(*N-B*)aminoborane
 aminoborane(*N-B*)trifluoroborane
 trimethylamine(*N-B*)methyl-
 (methylamino)borane
O-methylhydroxylamine(*N-B*)borane
 dicyclopentadienyldihydridotungsten-
 (*W-B*)trifluoroborane
 methylamine(*N-C*)-7-carba-*nido*-
 undecaborane
 (For numbering see *Figure 1*)

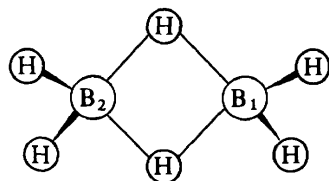
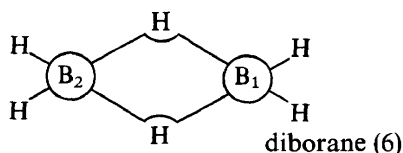
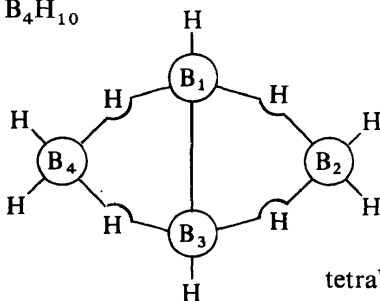


Figure 1.



tetraborane (10)

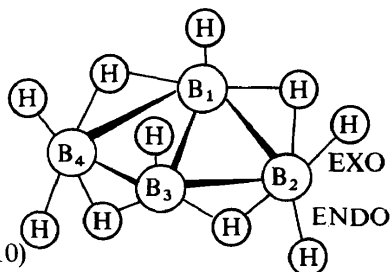


Figure 2.

endo-2,4-ethylenetetraborane(10)

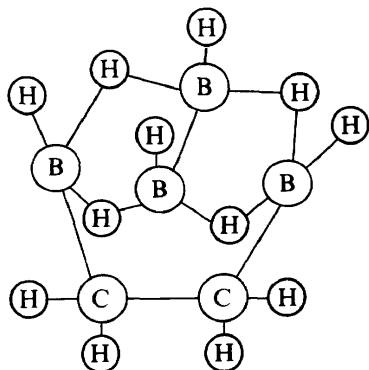


Figure 2a.

NOMENCLATURE OF INORGANIC BORON COMPOUNDS

B_5H_9

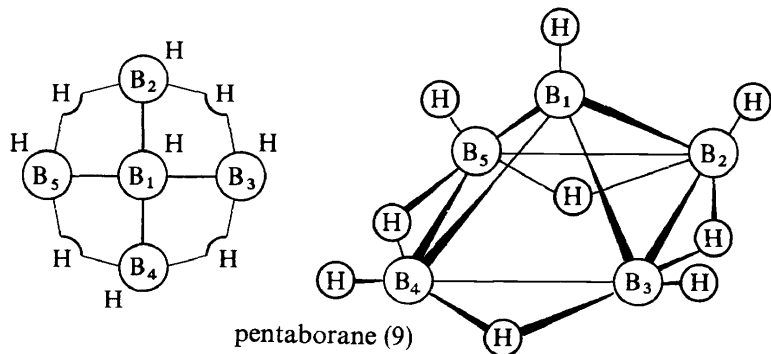


Figure 3.

B_5H_{11}

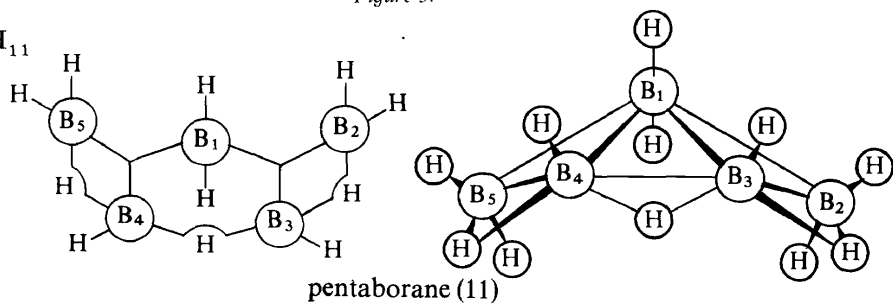


Figure 4.

B_6H_{10}

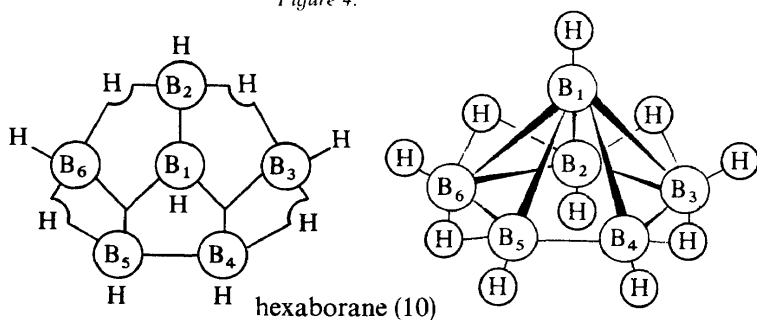


Figure 5.

B_8H_{12}

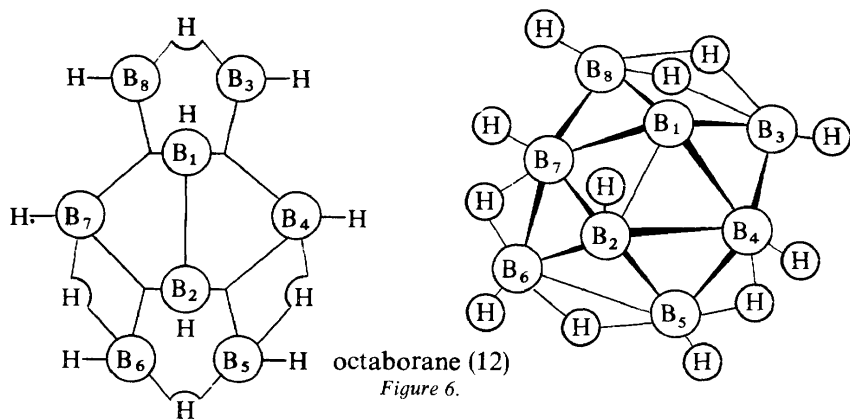
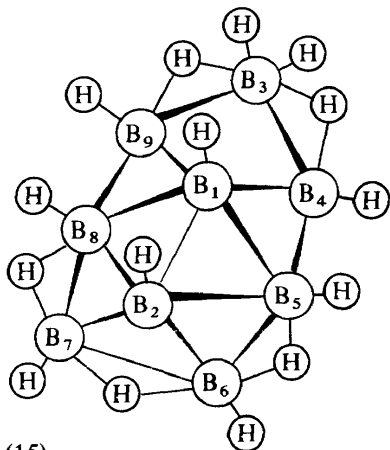
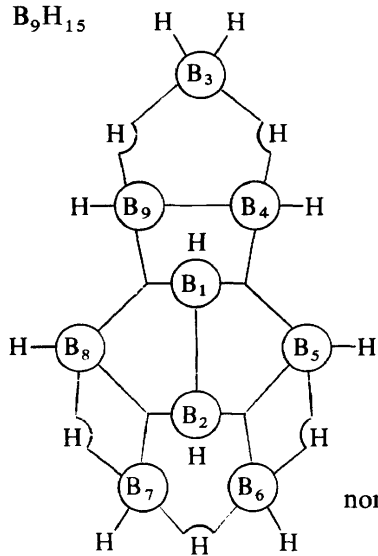


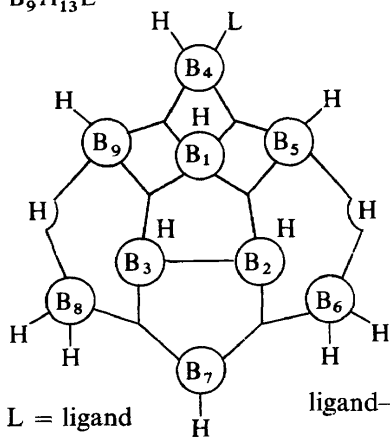
Figure 6.

NOMENCLATURE OF INORGANIC BORON COMPOUNDS



nonaborane (15)

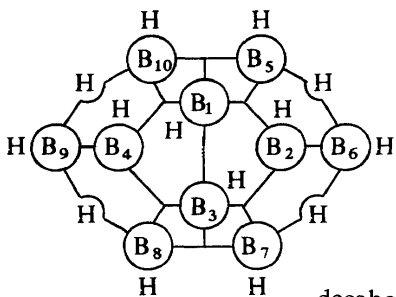
Figure 7.



L = ligand

ligand-nonaborane (13)

Figure 8.



decaborane (10)

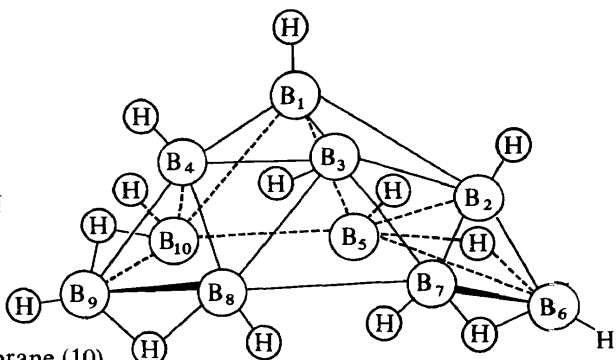
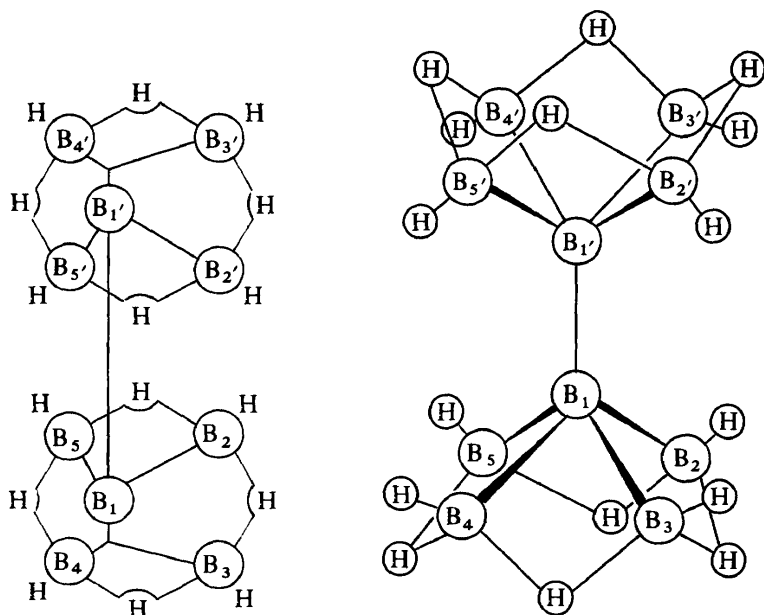


Figure 9.

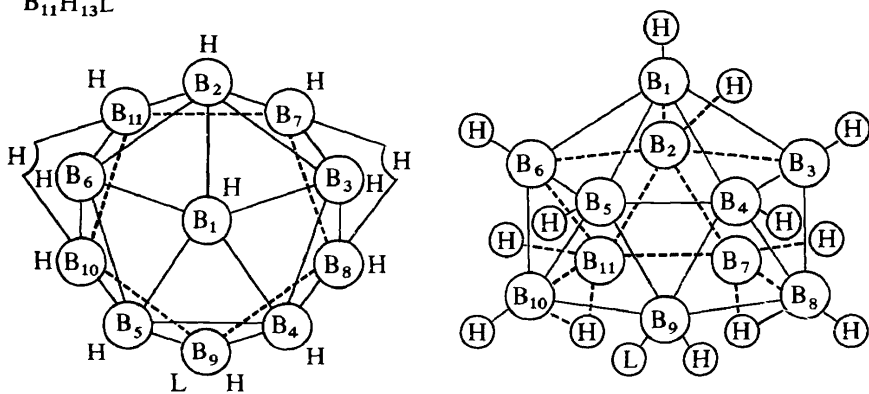
$B_{10}H_{16}$



decaborane (16)

Figure 10.

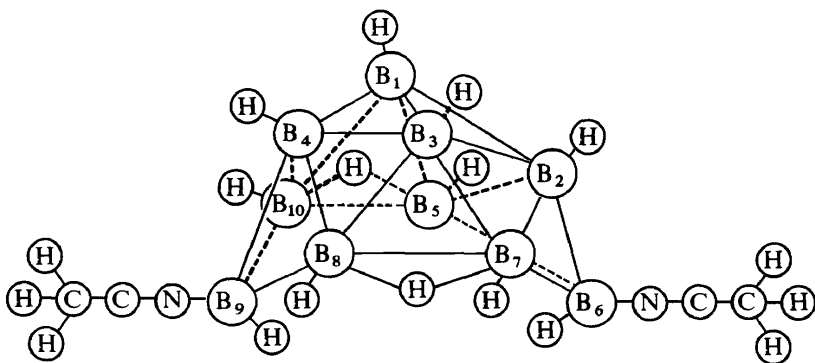
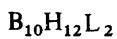
$B_{11}H_{13}L$



nido-undecaborane (13)
with attached ligand

Figure 11.

NOMENCLATURE OF INORGANIC BORON COMPOUNDS



exo-bis(acetonitrile) decaborane(12)

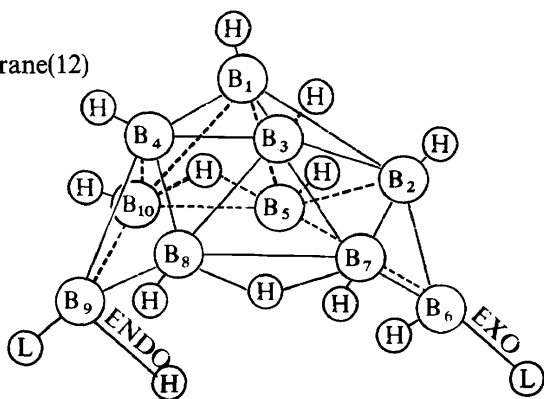
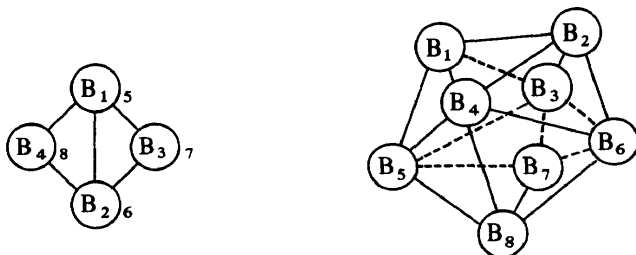


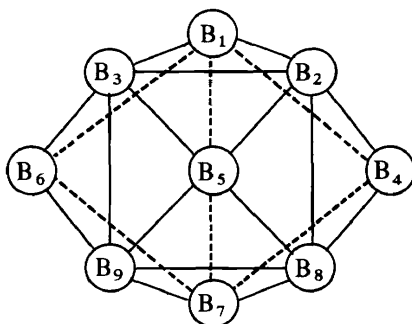
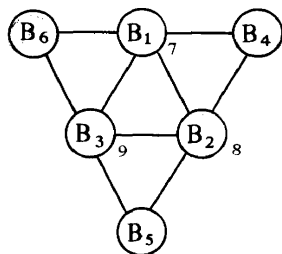
Figure 12.



closo-octaborane(8) skeleton
(dodecahedron)

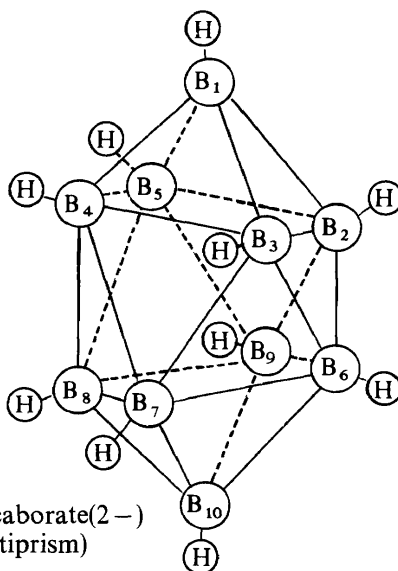
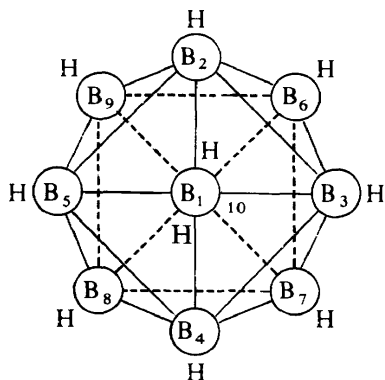
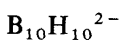
Figure 13.

NOMENCLATURE OF INORGANIC BORON COMPOUNDS



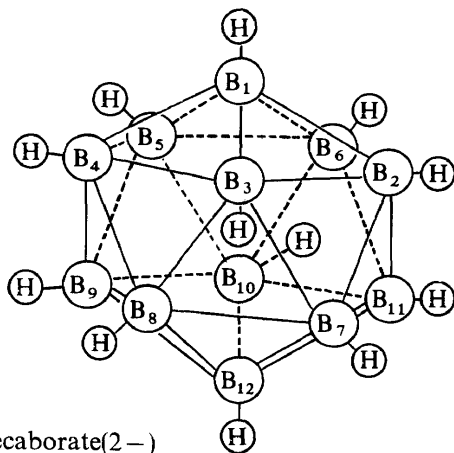
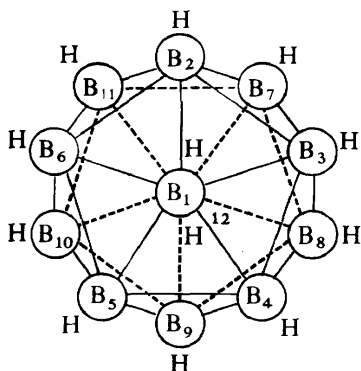
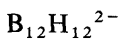
closo-nonaborane skeleton
(tricapped trigonal prism)

Figure 14.



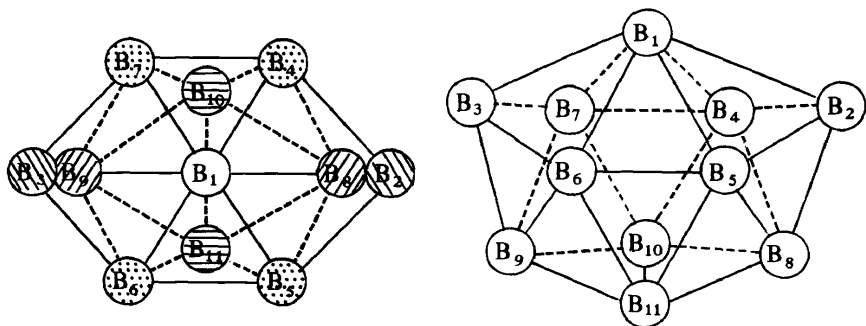
decahydro-*closo*-decaborate(2-)
(bicapped square antiprism)

Figure 15.



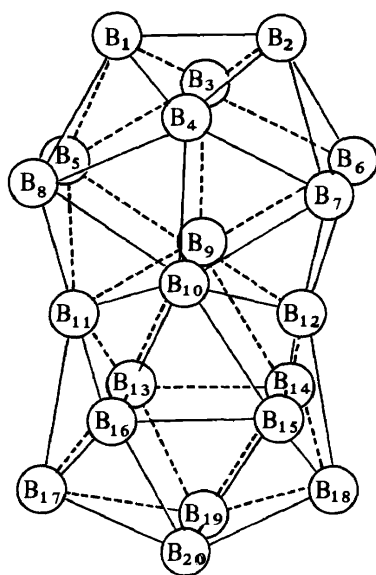
dodecahydro-*closo*-dodecaborate(2-)
(icosahedron)

NOMENCLATURE OF INORGANIC BORON COMPOUNDS



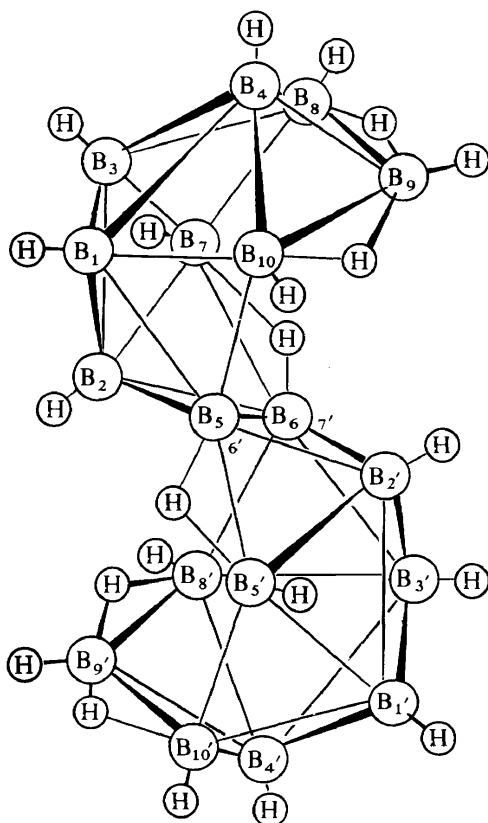
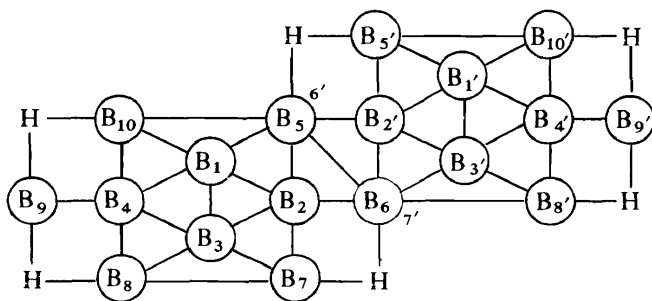
closo-undecaborane skeleton

Figure 17.



closo-icosaborane(16) skeleton

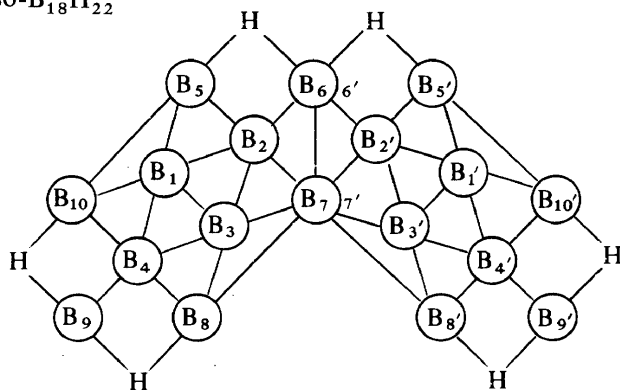
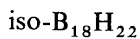
Figure 18.



octadecaborane (22)

Figure 19a.

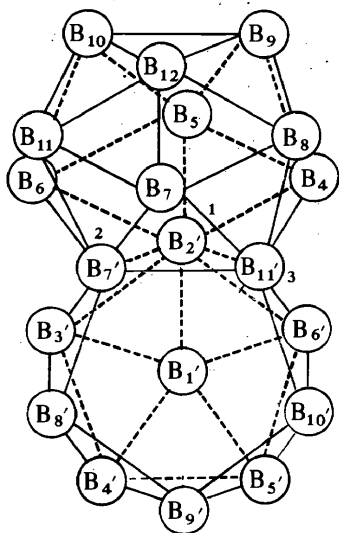
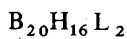
NOMENCLATURE OF INORGANIC BORON COMPOUNDS



The enantiomer is fused at the (5',6';5,6) position.

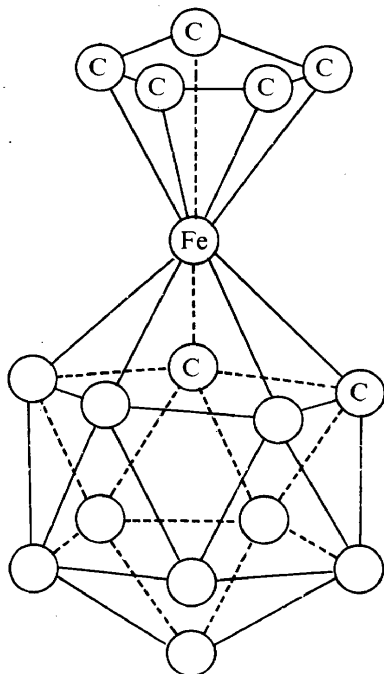
octadecaborane(22) isomer

Figure 19b.



nido-undecaborano[2',7',11';1,2,3]-closo-dodecaborane skeleton

Figure 20.



3- η -cyclopentadienyl-1,2-dicarba-3-ferra-closo-dodecaborane skeleton

Figure 21.

NOMENCLATURE OF INORGANIC BORON COMPOUNDS

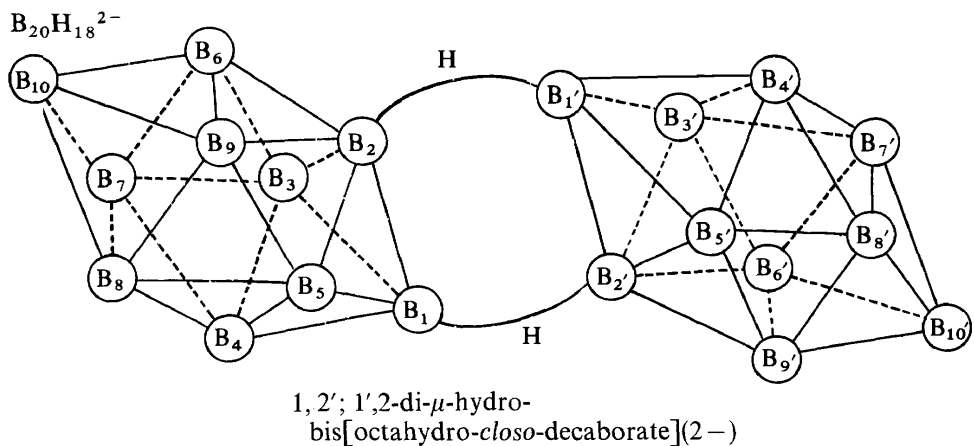


Figure 22.

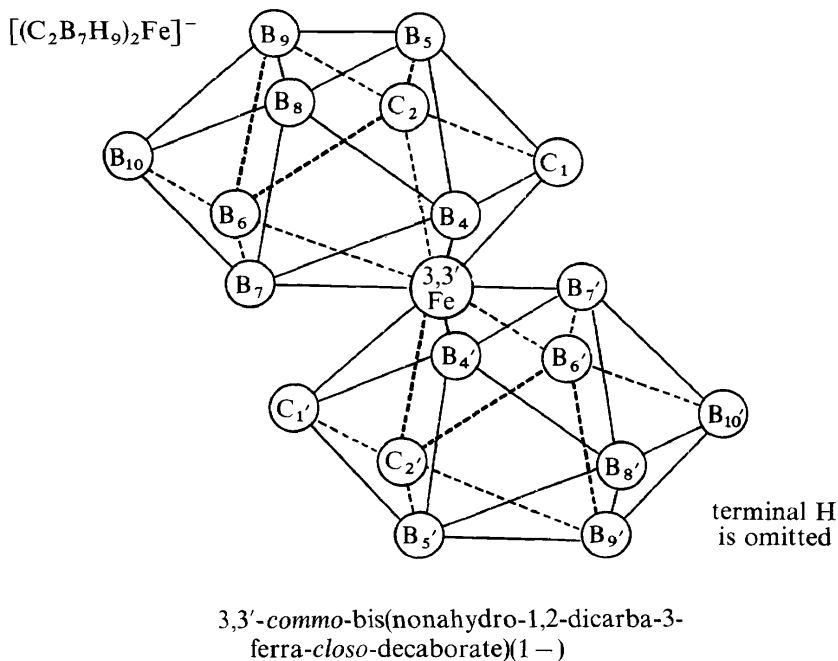


Figure 23.

REFERENCES

- ¹ International Union of Pure and Applied Chemistry. *Nomenclature of Inorganic Chemistry*. 2nd ed. Butterworths: London (1971). (a) **Rule 2.251**; (b) **Rules 5.213 and 5.214**; (c) **Rule 7.711**; (d) **Rule 7.52**; (e) **Rule 7.611**; (f) **Rule 7.514**; (g) Section 7; (h) **Rule 2.252**; (i) **Rule 4.1**; (j) **Rule 7.42**.
- ² International Union of Pure and Applied Chemistry. *Nomenclature of Organic Chemistry*. 3rd ed. Butterworths: London (1971). (a) **Rule A-52**; (b) **Rules A-21.3 and B-3**; (c) **Rule C-10.1**; (d) **Rule B-1.4**; (e) **Rule B-1**; (f) **Rules B-4 and C-0.6**.
- ³ *Inorg. Chem.* **2**, 1087 (1963).