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Inorganic Chemistry

The Nomenclature of Boron Compounds

The following rules for the nomenclature of boron compounds have been approved by the Council of the American Chemical Society. As a result of the Council's action, these rules are tentative for 1 year before becoming official nomenclature policy of the American Chemical Society. Comments on these rules are solicited and should be sent to either Dr. Roy M. Adams, Geneva College, Beaver Falls, Pa. 15010, or Dr. Kurt L. Loening, Chemical Abstracts Service, The Ohio State University, Columbus, Ohio 43210.

Historical

The first proposals for a set of rules for naming boron compounds arose from the work of several informal groups concerned with the rapid development in boron chemistry during the early 1950's. This early work was summarized in a paper[1] which was subsequently reviewed in some detail.[2]

These activities led to the establishment of the Advisory Subcommittee on the Nomenclature of Boron Compounds to the Nomenclature Committee of the American Chemical Society Division of Organic Chemistry. The advisory subcommittee, under the chairmanship of Dr. Kurt L. Loening, submitted a report on boron nomenclature in 1958. This report was reviewed and referred back to the advisory subcommittee for revision. At this time the Division of Inorganic Chemistry of the American Chemical Society was formed. The Advisory Subcommittee on the Nomenclature of Boron Compounds was reconstituted as a subcommittee of the Inorganic Division's nomenclature committee. Because of the rapid development of research dealing with cage boron compounds, a large amount of work was necessary to develop rules for naming such structures.[3]

The present set of rules is largely due to the efforts of Dr. James Carter, who was appointed chairman of the Boron Subcommittee in 1964. Four separate and complete drafts have been prepared, each of which has been widely circulated to interested parties for comment and criticism. The rules given below were approved by the Inorganic Nomenclature Subcommittee of the National Academy of Sciences—National Research Council, Miss Janet D. Scott, chairman, in August 1967; by the Nomenclature Committee of the ACS Division of Inorganic Chemistry, Dr. Roy M. Adams, chairman, in September 1967; by the ACS Committee on Nomenclature, Dr. Kurt L. Loening, chairman, in November 1968; and by the Council of the American Chemical Society in April 1968.

Introduction

There are certain bonding situations common in boron chemistry and uncommon elsewhere that lead to unusual nomenclature problems. These include the following:

excess connectivity or ligancy. In elemental boron each atom has six or seven nearest neighbors. With other elemental nonmetals the number of nearest neighbors 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 traditional 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 neighbors, but for them some relatively fluid "electron glue" is assumed with no directional character. 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 20 faces (which in this case are equilateral triangles), 17 vertices (occupied in this case by 12 boron atoms), and 30 edges (or connections between atoms). This icosahedral framework is apparently held together by 26 electrons, again pointing up the nontraditional bonding.

The nomenclature problem is compounded by the *formation of many molecular hydrides.* Boron forms more known molecular hydrides than any other element except carbon. Most of these have boron skeletons which can be viewed as fragments of an icosa-

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(1) G. Schaeffer and T. Wartik, 125th National Meeting of the American Chemical Society, Kansas City, Mo., 1954.

(2) A. M. Patterson, *Chem. Eng. News*, **32**, 1441 (1954); **34**, 560 (1956).

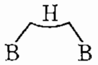
(3) R. M. Adams, *Inorg. Chem.*, **2**, 1087 (1963).

hedron. In the neutral hydrides the open edges of the fragments are generally "sewed up" by

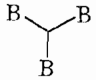
bridged hydrogens. In the "open" boron hydrides there are at the edges of the molecule some hydrogens connected to two borons, a phenomenon largely unknown in the chemistry of other elements. There are also

unusual fusions. The isosahedral 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-center bonds* (*i.e.*, a pair of electrons being shared among three atoms). Hence, a standard representation for a three-center bond is convenient, as is a line for a two-center bond. Those commonly used are



for a hydrogen bridge and



for a three-centered bond involving only boron atoms. However, for elemental boron and for all but the two simplest boron hydrides, several equally valid three-center 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-center bonds is inadequate in all but the simplest boron compounds.

Negative Formal Charge. In many stable boron-containing particles, the particle has extra electrons beyond those that it and other bonded atoms can contribute: *e.g.*, in $\mathrm{BH_4^-}$, isoelectronic with methane, and in $\mathrm{B_{12}H_{12}^{2-}}$, which contains the icosahedron referred to above. The last particle appears to have more derivative possibilities 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.*, $\mathrm{B_{12}H_9(NH_3)_3^+}$. Also, replacement of boron atoms by other nonmetal atoms (stripped to three valence electrons to be isoelectronic with boron) forms neutral and cationic replacement derivatives of the boron hydride anions; *e.g.*, $\mathrm{B_{10}C_2H_{12}}$, $\mathrm{B_{11}PH_{12}}$, and $\mathrm{B_{11}SH_{12}^+}$. All these examples have skeletons isoelectronic with $\mathrm{B_{12}H_{12}^{2-}}$. Such skeletons are conveniently named by postulating *unknown parent species.* (See Rules 1.4, 4, and 6.) In the nomenclature of other elements this occurs rather rarely (*e.g.*, orthocarbonic acid), but in the chemistry of boron it is commonplace.

To recapitulate, boron forms more known volatile hydrides than any other element, except carbon, and has a corresponding many-faceted chemistry. Nearly all the precedents and suggestions for nomenclature of such structures have been based on carbon chemistry. However, the bonding and structures are evidently quite different from those in carbon compounds.

The most stable boron-containing particles are anions for which the nomenclature precedents nearly all come from inorganic coordination nomenclature.

With this borderline element, two types of precedent exist, and the extra phenomena mentioned above require novel approaches to nomenclature.

Index to Rules

Rules

Rule 1. Boron Hydrides

1.1.—The combining form of boron is "bor-" and this is used to designate the presence of boron.

Example:

$\mathrm{BH_3}$	borane

Note.—It must be recognized that there will be modifications of the simple bor- in practice:

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

1.2.—The term "borane" is used to designate compounds of boron and hydrogen.

1.3.—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 *icosa* rather than *eicosa* to agree with common practice in geometry as opposed to the practice in organic hydrocarbon nomenclature.)

1.4.—The number of hydrogen atoms in the molecule is indicated by enclosing the appropriate Arabic numeral in parentheses directly following the name. Alternatively, the number followed by a lower case h without a space is placed at the end of the name and separated by a hyphen.

Examples:

(1)	BH	borane(1) or borane-1h
(2)	$\mathrm{BH_3}$	borane(3) or borane-3h
(3)	B_2H_4	diborane(4) or diborane-4h
(4)	$\mathrm{B_2H_6}$	diborane(6) or diborane-6h (Figure 1)
(5)	B_3H_7	triborane(7) or triborane-7h
(6)	B_4H_4	tetraborane(4) or tetraborane-4h
(7)	B_4H_8	tetraborane(8) or tetraborane-8h
(8)	$\mathrm{B_4H_{10}}$	tetraborane(10) or tetraborane-10h (Figure 2)
(9)	B_5H_5	pentaborane(5) or pentaborane-5h
(10)	$\mathrm{B_5H_9}$	pentaborane(9) or pentaborane-9h (Figure 3)
(11)	$\mathrm{B_5H_{11}}$	pentaborane(11) or pentaborane-11h (Figure 4)

(12)	B_6H_6	hexaborane(6) or hexaborane-6h
(13)	$\mathrm{B_6H_{10}}$	hexaborane(10) or hexaborane-10h (Figure 5)
(14)	$\mathrm{B_6H_{12}}$	hexaborane(12) or hexaborane-12h
(15)	B_7H_7	heptaborane(7) or heptaborane-7h
(16)	B_8H_8	octaborane(8) or octaborane-8h
(17)	$\mathrm{B_8H_{12}}$	octaborane(12) or octaborane-12h (Figure 6)
(18)	B_9H_9	nonaborane(9) or nonaborane-9h
(19)	B_9H_{13}	nonaborane(13) or nonaborane-13h
(20)	$\mathrm{B_9H_{15}}$	nonaborane(15) or nonaborane-15h (Figure 7)
(21)	$B_{10}H_8$	decaborane(8) or decaborane-8h
(22)	$B_{10}H_{12}$	decaborane(12) or decaborane-12h
(23)	$\mathrm{B_{10}H_{14}}$	decaborane(14) or decaborane-14h (Figure 9)
(24)	$\mathrm{B_{10}H_{16}}$	decaborane(16) or decaborane-16h (Figure 10)
(25)	$B_{11}H_{11}$	undecaborane(11) or undecaborane-11h
(26)	$B_{11}H_{13}$	undecaborane(13) or undecaborane-13h
(27)	$B_{12}H_{10}$	dodecaborane(10) or dodecaborane-10h
(28)	$\mathrm{B_{18}H_{22}}$	octadecaborane(22) or octadecaborane-22h (Figure 19)
(29)	$\mathrm{B_{20}H_{16}}$	icosaborane(16) or icosaborane-16h (Figure 18)

Note.—Those hydrides whose formulas are given in italics are known only in the form of derivatives or adducts (see Rules 2 and 6). These names are based on molecular formulas rather than structures. Inclusion of sufficient information to unambiguously define structure would lead to extremely complex names. See the figures in the Appendix.

Comments.—(1) ACS Nomenclature Committees prefer the parentheses to avoid confusion with locants at the end of radical names (see Rule 3.4). The IUPAC Inorganic Nomenclature Commission currently prefers the hyphenated suffix, followed by the lower case h if necessary to avoid ambiguity, feeling that this causes less possibility of confusion with references.

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

Examples:

(1)	$\mathrm{BH_3}$	borane
(2)	$\mathrm{B_2H_6}$	diborane

(3) During the period when the differences in the structures of two or more isomers were not known the prefixes "iso-" and "neo-" have been used to distinguish isomers. Once structures are known, there is no need for this nomenclature.

Examples:

(1)	$\mathrm{B_{18}H_{22}}$	octadecaborane(22) (Figure 19)
(2)	iso-$\mathrm{B_{18}H_{22}}$	isooctadecaborane(22) (Figure 19)

1.41.—Boranes that may be considered to be formed by fusion or joining of simpler boranes may also be named as derivatives of the simpler boranes. (For numbering practices see Rules 2.32 and 2.331.)

Examples:

(1)	$\mathrm{B_{10}H_{16}}$	1,1′-bipentaborane(9) (Figure 10)
(2)	$\mathrm{B_{18}H_{22}}$	decaborano(14)[6′,7′:5,6]decaborane(14) (Figure 19)
(3)	iso-$\mathrm{B_{18}H_{22}}$	decaborano(14)[6′,7′:6,7]decaborane(14) (Figure 19)

Comment.—Examples (2) and (3) are fusion type names.[4a] When the fusion involves only one atom, the prefix *commo* (for common atom from Latin *communis* or common) is suggested. Currently known cases of this phenomenon involve a metal atom shared between two carbaborane or thiaborane cages (see Rules 4.3 and 7.5). Such a prefix is necessary to avoid confusion with compounds where an atom in one skeleton is directly bonded to an atom in another skeleton as in example (1) above. Spiro has a similar meaning in organic nomenclature and may be a better choice in the interest of uniformity, although the derivation is more ambiguous.

1.5.—In cases where the structures of isomeric boron hydrides are known, the isomers may be distinguished by adding a comma and the italicized Schoenflies symbol[5] of the highest symmetry element following the number of hydrogens in each name.

Examples:

(1)	$\mathrm{B_{18}H_{22}}$	octadecaborane(22,C_i) (Figure 19)
(2)	iso-$\mathrm{B_{18}H_{22}}$	octadecaborane(22,C_2) (Figure 19)

1.6.—The polyboranes and their derivatives may be considered to consist of two general classes: (1) closed structures (that is, structures with boron skeletons that are polyhedra having all triangular faces) and (2) nonclosed structures. The members of the first class are designated by the italic 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 italic prefix *nido*- is used.

Examples:

(1)	$\mathrm{B_4Cl_4}$	tetrachloro-*closo*-tetraborane(4)
(2)	$\mathrm{2[(CH_3)_2S]\cdot B_{10}H_8}$	bis(dimethyl sulfide)-*closo*-decaborane(8)[6]
(3)	$\mathrm{2[(CH_3)_2S]\cdot B_{10}H_{12}}$	bis(dimethyl sulfide)-*nido*-decaborane(12)[6]
(4)	$\mathrm{B_{10}H_{14}}$	*nido*-decaborane(14)
(5)	$\mathrm{B_{20}H_{16}}$	*closo*-icosaborane(16)

Note.—The need for these prefixes becomes more evident in naming hetero boranes and boron hydride anions (see Rules 4.1 and 7.4).

Comment.—The prefix *clovo*-[3] derived from the Greek word for cage was changed to *closo*- at the request of the IUPAC Inorganic Nomenclature Commission. The prefix *nido*- is derived from the Greek word for nest.

Rule 2. Derivatives of the Boranes

2.1.—Derivatives of borane, $\mathrm{BH_3}$, are named in the same manner as those of other simple hydrides.[7a]

Examples:

(1)	$\mathrm{Cl_2BH}$	dichloroborane
(2)	$\mathrm{H_2SbBH_2}$	stibinoborane

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(4) (a) International Union of Pure and Applied Chemistry, "Nomenclature of Organic Chemistry, Sections A and B," 2nd ed, Butterworths, London, 1966, p 5; (b) Section A; (c) Section B; (d) Section B, Rule B-1.

(5) W. H. Jaffe and M. Orchin, "Symmetry in Chemistry," John Wiley and Sons, Inc., New York, N. Y., 1965.

(6) Addition type names—see Rule 6.

(7) (a) International Union of Pure and Applied Chemistry, "Nomenclature of Inorganic Chemistry," Butterworths, London, 1959, Rule 2.3; (b) Rule 2.25; (c) Rule 7; (d) Rule 7.5.

(3)	Br_2BF	di*b*romo*f*luoroborane
(4)	Cl_2BI	di*c*hloro*i*odoborane
(5)	$(CH_3)_2BBr$	*b*romodi*m*ethylborane
(6)	$BH(OCH_3)_2$	dimethoxyborane
(7)	$B(CH_3)_3$	trimethylborane
(8)	$ClB(OCH_3)_2$	*c*hlorodi*m*ethoxyborane
(9)	$CH_3OB(CH_3)_2$	*metho*xydi*methy*lborane[8]
(10)	$(CH_3)_2BOH$	*h*ydroxydi*m*ethylborane[8]
(11)	$(CH_3)_2BC_3H_7$	di*m*ethyl*p*ropylborane
(12)	Cl_2BCH_3	di*c*hloro*m*ethylborane
(13)	$Cl_2BCH_2CH_2BCl_2$	ethylenebis[dichloroborane]
(14)	$(CH_3)_2BOB(CH_3)_2$	oxybis[dimethylborane]
(15)	$[(CH_3)_2N]_2BH$	bis(dimethylamino)borane
(16)	$(CH_3)_2NB(CH_3)_2$	(*d*imethylamino)di*m*ethylborane

Note.—The substituents are listed alphabetically. The critical letters are italicized in the above examples to permit ready recognition of the alphabetical order. Note also the use of multiplicative prefixes and enclosing marks for complex expressions. Borane takes enclosing marks as the root name over other nonmetallic functional groups. This is in harmony with the practice for organometallic and metal–metal bonded compounds[9d] in which precedence for its center of coordination is assigned to the element farther to the left in the periodic table and within families to the element lower in the family. However, Chemical Abstracts Service has now assigned borane a position in its order of precedence of functions, and derivatives of borane are named accordingly in the *Chemical Abstracts* Indexes.

2.2.—Binary boron compounds may also be named by the recognized practices for such compounds.[7b]

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}	aluminum dodecaboride
(6)	$B_{12}C_3$	dodecaboron tricarbide
(7)	CaB_6	calcium hexaboride

2.3.—Derivatives of the polyboron hydrides (polyboranes). Compounds that may be conceived as derived from a boron hydride by substitution of an atom or group for hydrogen are named as substitution derivatives with the name of the parent hydride as given in Rules 1.4 and 1.6.

2.31.—When a polyboron hydride 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 substituted boranes retain the original numerical suffix.

Examples:

(1)	$B_2(OCH_3)_4$	tetramethoxydiborane(4)
(2)	$B_2(OCH_3)_2(C_6H_5)_2$	dimethoxydiphenyldiborane(4)
(3)	B_2H_5Cl	chlorodiborane(6)
(4)	$B_{10}H_4I_{10}$	decaiododecaborane(14)

2.32.—Numbering of positions in open boron frameworks. For the use of *nido-*, see Rule 1.6.

2.321.—The boron atoms are numbered following plane projection drawings of the hydride structures viewed from opposite the open portion of the framework. The interior atoms in the projection are numbered first, followed by the peripheral atoms. Each set is numbered clockwise starting at 12 o'clock on the drawing or at the first position clockwise therefrom. If a choice exists, the drawing should be oriented so that the first (or earliest) position to be numbered occupies the 12 o'clock position. If the addition of only one atom will produce a closo structure having more than three planes of atoms perpendicular to the highest symmetry axis, the numbering for closo structures is used (see Figure 11 and Rule 2.331).

Example:

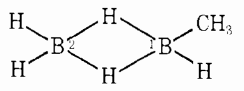
B_5H_9 considered as resting on the base (see Figure 3)

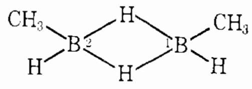
2.322.—If the orientation of the molecule is critical in assigning position numbers, the projection is aligned so that the symmetry plane containing the smallest number of atoms separated by the smallest distance is in the 12 to 6 o'clock position (*e.g.*, B_4H_{10}, Figure 2; $B_{10}H_{14}$, Figure 9). If a choice remains, the portion of the molecule with the most atoms in this symmetry plane is oriented to the top of the drawing (*e.g.*, B_5H_{11}, Figure 4; B_6H_{10}, Figure 5; $B_9H_{13}L$ (L = ligand), Figure 8). If a choice still remains, the portion of the molecule with the greatest number of bridge hydrogens is oriented to the botton of the drawing (*e.g.*, B_8H_{12}, Figure 6; B_9H_{15}, Figure 7).

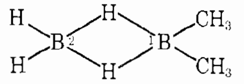
2.323.—In general the use of symbols and numbers follows standard practices of organic nomenclature.[4b,4c,10a] Additional practices are introduced in Rule 1.4 and the following rules.

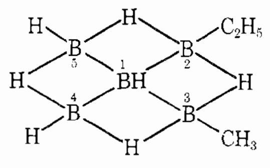
2.3231.—A nonbridging substitutional prefix is directly attached to the name of the parent compound and is numbered corresponding to the boron atom to which the substituent is attached.

Examples:

(1)

1-methyldiborane(6)

(2)

1,2-dimethyldiborane(6)

(3)

1,1-dimethyldiborane(6)

(4)

2-ethyl-3-methylpentaborane(9)

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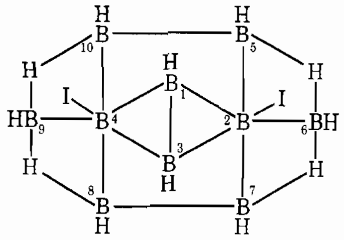
[8] In the past, compounds of this type have been regarded as boron acids and given names such as dimethylborinic acid.

[9] (a) International Union of Pure and Applied Chemistry, "Tentative Rules for Nomenclature of Inorganic Compounds, Section 7, Coordination Compounds," to be published; (b) Rules 7.412 and 7.414; (c) Rule 7.51; (d) Rule 7.521.

[10] (a) International Union of Pure and Applied Chemistry, "Nomenclature of Organic Chemistry," Section C, Butterworths, London, 1965; (b) Subsection C-0.6; (c) Rule 816.3.

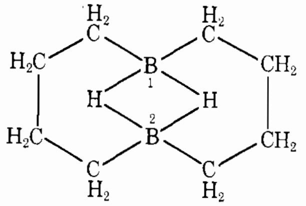
Note.—2-Ethyl-5-methylpentaborane(9) is the enantiomer numbered according to the pattern established for coordination compounds.[9b]

(5)



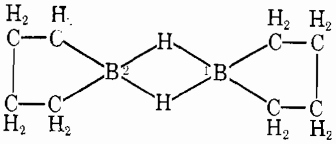
2,4-diiododecaborane(14) (see also Figure 9)

(6)



1,2:1,2-bis(tetramethylene)diborane(6)

(7)



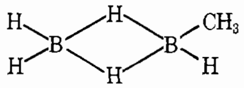
1,1:2,2-bis(tetramethylene)diborane(6)

Note.—It should be understood that the lines above do not imply conventional covalent bonds.

2.3232.—When it is desired to differentiate a terminal position from a bridging position, the symbol τ may be used.

Examples:

(1)



τ-methyldiborane(6)

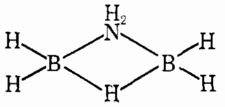
(2) $B_{10}H_4I_{10}$ deca-τ-iododecaborane(14)

2.3233.—Presently known boron hydrides containing BH_2 groups may be considered as fragments of an icosahedron. In such structures one hydrogen of the BH_2 group is directed away from the center 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 italic prefix "*exo-*" and the latter by the italic prefix "*endo-*" (see Figures 2, 2a, and 12).

2.3234.—Substituents in the bridge positions are designated by use of the symbol "μ-" as a prefix to the name of the substituent. 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. When bridging occurs between two boron skeletons, the lowest possible numbers are used to designate points of bridging as is done for substituents.

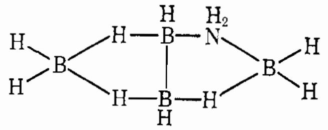
Examples:

(1)



μ-aminodiborane(6)

(2)



1,2-μ-aminotetraborane(10)

Note.—The second compound is the enantiomer of 2,3-μ-aminotetraborane(10).[9b]

The designation of bridging groups follows the pattern established for coordination compounds.[9c] Note that hydrogen bridges are not specifically designated.

2.33.—Closed boron frameworks. For use of *closo-*, see Rule 1.6.

2.331.—The boron atoms are numbered in sequential planes perpendicular to the longest highest-order axis. The atoms in each perpendicular plane are numbered clockwise from a reference plane through this symmetry axis. If there is a choice, that half of the symmetry axis with the greater number of atoms on this axis is numbered first. For cases where the orientation is critical, the molecule is viewed down this axis as a planar projection and oriented according to Rule 2.322 (*e.g.*, see Figure 17).

Rule 3. Radicals

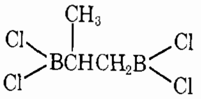
3.1.—Radicals derived from borane, BH_3, are named as follows:

H_2B—	boryl
Cl_2B—	dichloroboryl
$(CH_3)_2B$—	dimethylboryl
$(HO)_2B$—	dihydroxyboryl
OB—	oxoboryl
HB<	borylene
CH_3B<	methylborylene
HOB<	hydroxyborylene
B⋖	borylidyne

Note.—Boryl is used here and polyboranyl for polyboron radicals to avoid confusion with multiple $-BH_2$ groups. Thus, diboryl means two $-BH_2$ groups and diboranyl is the monovalent radical derived from diborane.

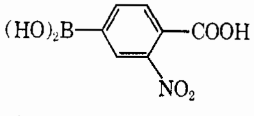
Examples:

(1)



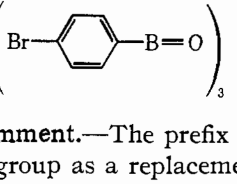
1,2-bis(dichloroboryl)propane or propylenebis[dichloroborane][11]

(2)



4-(dihydroxyboryl)-2-nitrobenzoic acid or (4-carboxy-3-nitrophenyl)dihydroxyborane[11]

(3)



1-bromo-4-(oxoboryl)benzene trimer or tris(4-bromophenyl)boroxin[11] (see Rule 5.3)

Comment.—The prefix borano has been used for the H_3B group as a replacement for oxygen in the naming of some anions.

Examples:

(1) $H_3BCO_2^{2-}$ boranocarbonate ion

(2) $H_2NC(BH_3)O^-$ boranocarbamate ion

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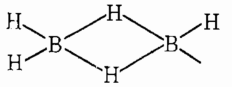
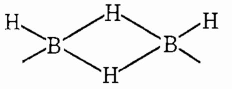
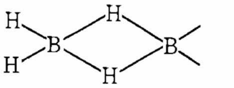
(11) Preferred name—see note under Rule 2.1.

3.2.—Radicals derived from boron hydrides containing two or more boron atoms may be named as follows:

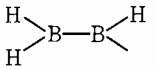

diboranyl

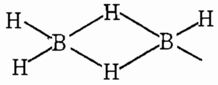

diboranylene

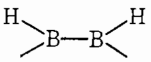

diboranylidene

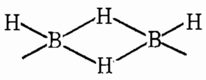
$—(B_{10}H_{12})—$ decaboranediyl

3.3.—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 hydrogens in the original hydride after the syllable "-an" and before the radical ending.

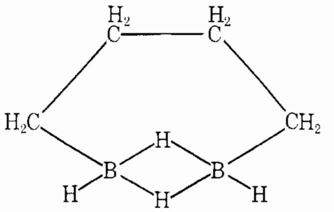
(1)

diboran(4)yl

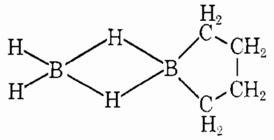
(2)

diboran(6)yl

(3)

diboran(4)ylene

(4)

diboran(6)ylene

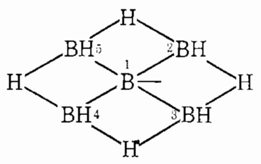
Examples:

(1)

1,4-diboran(6)ylenebutane or 1,2-tetramethylenediborane(6)[11]

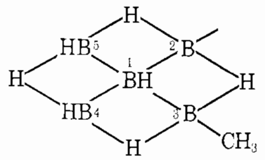
(2)

1,4-diboran(6)ylidenebutane or 1,1-tetramethylenediborane(6)[11]

3.4.—The position of attachment of a radical is indicated by placing the appropriate numeral or symbol before the radical name.

Examples:

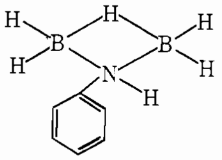
(1)

1-pentaboran(9)yl

(2) $(B_5H_8)_2CHCH_3$ 1,1-bis[1-pentaboran(9)yl]-ethane or 1,1′-ethylidene-bis[pentaborane(9)][11]

(3)

3-methyl-2-pentaboran(9)yl

Attachment of a radical at a bridging position is indicated by listing the atoms to which the bridge is attached, separated by a hyphen and enclosed in parentheses.

Example:


N-(1-2)diboranylaniline or *μ*-anilinodiborane(6)[11]

Rule 4. Boranes with Skeletal Replacement

4.1.—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, as carbaboranes, azaboranes, phosphaboranes, thiaboranes, etc.[4c,10b] In this adaptation, a BH group is replaced by an EH group where E is the replacing atom. For example, although there is no known stable neutral polyborane with twelve boron atoms, $B_{10}C_2H_{12}$ is very stable, has many known derivatives, and is named dicarbadodecaborane(12), as the dicarba replacement derivative of the unknown $B_{12}H_{12}$.

The prefixes "*closo*-" and "*nido*-" indicate closed and open networks as in Rule 1.6. 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 2.321, 2.322, and 2.331).

Comment.—In organic replacement nomenclature a methylene (CH_2) group is replaced 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.

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 1.4). In the hetero polyboranes the number of nearest neighbors 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 a BH group is only by an EH group.

Examples:

(1) $B_3C_2H_5$ dicarba-*closo*-pentaborane(5)
(2) $B_4C_2H_6$ 1,2-dicarba-*closo*-hexaborane(6)

(3) $B_4C_2H_6$	1,6-dicarba-*closo*-hexaborane(6)
(4) B_5CH_7	carba-*closo*-hexaborane(7)
(5) $B_4C_2H_8$	4,5-dicarba-*nido*-hexaborane(8) (for numbering see Figure 5)
(6) $B_5C_2H_7$	dicarba-*closo*-heptaborane (7)
(7) $B_6C_2H_8$	dicarba-*closo*-octaborane(8)
(8) $B_7C_2H_9$	dicarba-*closo*-nonaborane(9)
(9) $B_8C_2H_{10}$	dicarba-*closo*-decaborane(10)
(10) $B_9C_2H_{13}$	7,8-dicarba-*nido*-undecaborane(13) (for numbering see Figure 11)
(11) $CH_3NH_2 \cdot B_{10}CH_{10}$	methylamine(*N*–*C*)carba-*closo*-undecaborane(10)[6] or decahydro-*C*-(methylamine)carba-*closo*-undecaboron[12]
(12) $B_{10}C_2H_{12}$	1,2-dicarba-*closo*-dodecaborane(12) 1,7-dicarba-*closo*-dodecaborane(12) 1,12-dicarba-*closo*-dodecaborane(12) isomers (for numbering see Figure 16)
(13) $B_{11}PH_{12}$	phospha-*closo*-dodecaborane(12) (for numbering see Figure 16)
(14) $B_{10}CPH_{11}$	1-phospha-2-carba-*closo*-dodecaborane(11) (for numbering see Figure 16)
(15) $B_{10}SH_{12}$	7-thia-*nido*-undecaborane(12) (for numbering see Figure 11)

Comment.—Carborane has been used as a class name for the carbaboranes and also as a trivial name for $B_{10}C_2H_{12}$ and the isomers have been called *ortho*, *meta*, and *para*.

4.2.—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 (see Rule 4.1). Alternatively, they may be named as a nido ligand bonded to the metal atom.

Example:

$C_5H_5FeC_2B_9H_{11}$	3-π-cyclopentadienyl-1,2-dicarba-3-ferra-*closo*-dodecaborane(12) (Figure 21) or π-cyclopentadienyl-π-undecahydro-7,8-dicarba-*nido*-undecaboratoiron (see Rule 7.5)

Comment.—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 $B_7C_2H_{11}^{2-}$.

4.3.—When an atom is shared between two borane cages the prefix *commo* is suggested (see Rule 1.41).

Example:

$(B_9C_2H_{11})_2Ni$	3,3′-*commo*-bis[1,2-dicarba-3-nickela-*closo*-dodecaborane(11)]

Note.—See also Rule 7.5 and compare Figure 23.

4.4.—Radicals derived from hetero boranes are named by following the system described in Rule 3.

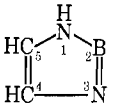
4.5.—Ions derived from hetero boranes are named by the principles of Rule 7.

Rule 5. Ring Systems

5.1.—Names for four-, five-, and six-membered rings, particularly in the lower stages of hydrogenation, are most conveniently named by the Hantzsch–Widman system[4d] and the practices established in "The Ring Index."[13]

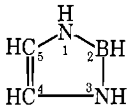
Examples:

(1)



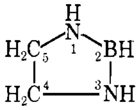
1*H*-1,3,2-diazaborole

(2)



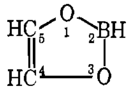
Δ^4-1,3,2-diazaboroline

(3)



1,3,2-diazaborolidine

(4)



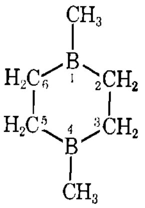
1,3,2-dioxaborole

Comment.—For the purposes of naming, the "lowest" state of hydrogenation is based on trivalency for both boron and nitrogen.

5.2.—Names for six-membered rings in the highest stage of hydrogenation and for larger rings, especially when they are in the highest stage of hydrogenation and contain isolated boron atoms, may be based on those of the saturated cyclic hydrocarbons utilizing replacement nomenclature. Hantzsch–Widman names[4d] and fusion names are also used for naming rings of this type.[13]

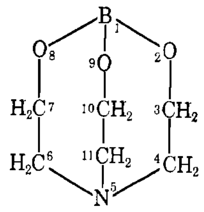
Examples:

(1)



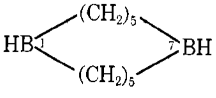
1,4-dimethyl-1,4-diboracyclohexane

(2)



2,8,9-trioxa-5-aza-1-borabicyclo-[3.3.3]undecane

(3)



1,7-diboracyclododecane

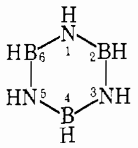
5.3.—There are a few ring systems containing boron that are particularly stable and consequently give rise to a considerable number of derivatives. Such rings usually arise from alternate boron atoms and atoms of group V or VI elements. Trivial names for these have been widely used and are retained.

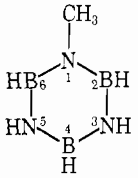
---

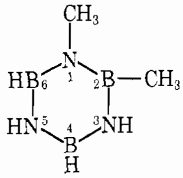
(12) Coordination type name, see Rule 7.

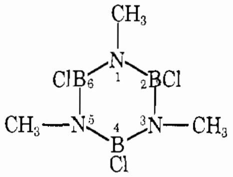
(13) A. M. Patterson, L. T. Capell, and D. F. Walker, "The Ring Index," 2nd ed, American Chemical Society, Washington, D. C., 1960.

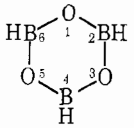
Examples:

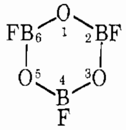
(1)

borazine

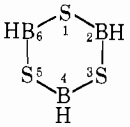
(2)

1-methylborazine

(3)

1,2-dimethylborazine

(4)

2,4,6-trichloro-1,3,5-trimethylborazine

(5)

boroxin

(6)

trifluoroboroxin

(7)

borthiin

Comment.—One of the most difficult problems in inorganic nomenclature involves description of rings and chains with elements having "unusual" coordination numbers, *e.g.*

$$(\overset{-}{B}H_2\overset{+}{N}H_2)_3,\ (\overset{-}{B}H_2\overset{+}{P}H_2)_4,\ \text{and}\ (\overset{+}{P}X_2\overset{-}{N})_4$$

At present, these compounds are probably best named as oligomers of the monomeric species having ordinary coordination numbers, *e.g.*, aminoborane cyclic trimer. The trivial names given above are recommended for the cyclic oligomers having ordinary coordination numbers.

Rule 6. Addition Compounds

A large number of boron-containing compounds may be considered formally as the union of a neutral Lewis base (electron-pair donor or nucleophile) with a boron compound (Lewis acid or electron-pair acceptor or electrophile). Hence they are named as addition compounds even though some of them are not formed in this simple fashion.

6.1.—The base and acid molecules are each given their proper names with the base first, and joined by a dash.

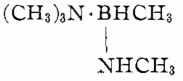
6.2.—The number of hydrogens in the borane or polyborane parent structure (known or postulated) is given the appropriate Arabic numeral in the customary manner.

Examples:

(1) $(CH_3)_3N \cdot BH_3$	trimethylamine–borane
(2) $(CH_3)_3N \cdot B_3H_7$	trimethylamine–triborane(7)
(3) $2CH_3CN \cdot B_{10}H_{12}$	*exo*-6,9-bis(acetonitrile)–decaborane(12) (see Figure 12)
(4) $2NH_3 \cdot B_{12}H_{10}$	diammine–dodecaborane(10)
(5) $2C_2H_5NH_2 \cdot B_5H_9$	bis(ethylamine)–pentaborane(9)
(6) $2N_2 \cdot B_{12}H_{10}$	bis(dinitrogen)–dodecaborane(10)
(7) $2(CH_3)_2S \cdot B_{10}Cl_6H_2$	bis(dimethyl sulfide)–hexachlorodecaborane(8)

6.3.—If there are possible alternatives in the manner of attachment of the base to the acid or when it is desired to emphasize the manner of attachment, the dash is replaced by parentheses enclosing the italicized symbols of the two elements forming the base-to-acid bond separated by a dash.

Examples:

(1) $OC \cdot BH_3$	carbon monoxide(*C–B*)borane
(2) $(CH_3)_3N \cdot BH_2NH_2$	trimethylamine(*N–B*)aminoborane
(3) $BH_2NH_2 \cdot BF_3$	aminoborane(*N–B*)trifluoroborane
(4)  $(CH_3)_3N \cdot \underset{\substack{\vert \\ NHCH_3}}{BHCH_3}$	trimethylamine(*N–B*)methyl-(methylamino)borane
(5) $CH_3ONH_2 \cdot BH_3$	*O*-methylhydroxylamine(*N–B*)borane[11] or methoxyamine(*N–B*)borane
(6) $(C_5H_5)_2H_2W \cdot BF_3$	dicyclopentadienyldihydrotungsten(*W–B*)trifluoroborane

Rule 7. Ions Related to Boron Hydrides

7.1.—Boron-containing ions and their salts may be named according to the rules for naming coordination compounds.[7c,9a] Following the American recommendations, "hydro-" is used in preference to "hydrido-." The nature of the hydrogens in boron hydrides varies from hydridic (or negative) in diborane(6) to protonic (or positive) in the moderately strong acid decaborane(14). Thus, it is impractical in boron nomenclature to systematically include information on the type of hydrogen.

Examples:

(1) $NaBF_4$	sodium tetrafluoroborate
(2) $LiBH_4$	lithium tetrahydroborate
(3) $Th(BH_4)_3$	thorium tris(tetrahydroborate)
(4) $NH_4[B(C_6H_5)_4]$	ammonium tetraphenylborate
(5) $[(CH_3)_4N][BCl_4]$	tetramethylammonium tetrachloroborate

Note.—The prefix "tetra-" may be dropped if no ambiguity results.

Examples:

(6) $NaBF_4$	sodium fluoroborate
(7) $LiBH_4$	lithium hydroborate

7.2.—In cases where the charge of the particle (or the oxidation state of the boron) is in question, the Ewens–Bassett convention is considered preferable to an indication of oxidation state, since fractional "Stock Numbers" would have to be used for the polyboron ions (see following rules).

Examples:

(1) $Na[BH_3CN]$	sodium cyanotrihydroborate(1−)
(2) $Ca[BH(CH_3)_2]$	calcium hydrodimethylborate(2−)
(3) $[H_2B(NH_3)_2]Cl$	diamminedihydroboron(1+) chloride
(4) $[(H_3B)_2Re(CO)_5]^-$	bis(borane)pentacarbonylrhenate(1−) ion
(5) $Ba[B(OH)_2F_2]_2$	barium difluorodihydroxyborate(1−)
(6) $K_2[Zn_3(BH_4)_8]$	potassium octakis(tetrahydroborato)-trizincate(2−)

7.3.—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 isopolyanions.[7d] Neutral derivatives may be named by this system or by addition nomenclature (see Rule 6).

Examples:

(1) $Na[B_2H_7]$	sodium heptahydrodiborate(1−)
(2) $Na_2[B_2(C_6H_5)_6]$	sodium hexaphenyldiborate(2−)
(3) $Ca[B_3H_8]_2$	calcium octahydrotriborate(1−)
(4) $Na[B_9H_{14}]$	sodium tetradecahydrononaborate(1−)
(5) $Na_2[B_{10}Cl_{10}]$	sodium decachlorodecaborate(2−)
(6) $Na_2[B_{10}H_{10}]$	sodium decahydrodecaborate(2−)
(7) $Na[B_{10}H_9NH_3]$	sodium amminenonahydrodecaborate(1−)
(8) $B_{10}H_8(NH_3)_2$	diammineoctahydrodecaboron
(9) $[B_{10}H_7(NH_3)_3]^+$	triammineheptahydrodecaboron(1+) ion
(10) $[B_{10}H_8(COOH)_2]^{2-}$	dicarboxyoctahydrodecaborate(2−) ion

7.4.—Prefixes, such as "*nido-*" and "*closo-*" for open and closed boron frameworks, respectively, may be used when required for clarity, as in Rule 1.6.

Examples:

(1) $Na_2[B_{10}H_{10}]$	sodium decahydro-*closo*-decaborate(2−)
(2) $Na_2[B_{10}H_{12}]$	sodium dodecahydro-*nido*-decaborate(2−)
(3) $Na[B_{10}H_{13}]$	sodium tridecahydro-*nido*-decaborate(1−)
(4) $Na_2[B_{10}H_{14}]$	sodium tetradecahydro-*nido*-decaborate(2−)
(5) $Na[B_{10}H_{15}]$	sodium pentadecahydro-*nido*-decaborate(1−)
(6) $[B_{12}H_{12}]^{2-}$	dodecahydro-*closo*-dodecaborate(2−) ion
(7) $[B_{12}H_{11}Cl]^{2-}$	chloroundecahydro-*closo*-dodecaborate(2−) ion
(8) $[B_{12}H_{11}NH_3]^-$	ammineundecahydro-*closo*-dodecaborate(1−) ion
(9) $B_{12}H_{10}(NH_3)_2$	diamminedecahydro-*closo*-dodecaboron

7.5.—Ions containing skeletal heteroatoms are named by the principles of this rule and Rule 4.

Examples:

(1) $[B_{11}H_{11}CH]^-$	dodecahydrocarba-*closo*-dodecaborate(1−)
(2) $[B_7C_2H_9]^{2-}$	nonahydrodicarba-*nido*-nonaborate(2−)
(3) $[(CO)_3ReB_9C_2H_{11}]^-$	3,3,3-tricarbonylundecahydro-1,2-dicarba-3-rhena-*closo*-dodecaborate(1−)
(4) $[Fe(B_7C_2H_9)_2]^-$	3,3′-*commo*-bis[nonahydro-1,2-dicarba-3-ferra-*closo*-decaborate](1−) (see Figure 23)

Comment.—Some German and British workers use the term boranate for boron hydride anions. Many American chemists have indicated a desire for such a system, largely on a basis of euphonics. Along with this is a desire for the use of substitution nomenclature for derivatives; for example there is an extensive derivative chemistry of the *closo* anions. However, 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 proposed.

7.6.—Zwitterions.—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 zwitterion molecules. These are best named as substituted borate anions or as borato derivatives of hydrocarbons.[10c]

Examples:

(1) $(H_3C)_3\overset{+}{P}CH_2\overset{-}{B}H_3$	trihydro[(trimethylphosphonio)-methyl]borate[11] or (trihydroborato)(trimethylphosphonio)methane
(2) $Cl_3\overset{+}{P}C_6H_4\overset{-}{B}Cl_3$	trichloro[(trichlorophosphonio)-phenyl]borate[11] or (trichloroborato)(trichlorophosphonio)-benzene

Acknowledgments.—Many individuals have contributed to the development of these rules. While there are too many to be cited individually, all contributions are gratefully acknowledged. The late Dr. George W. Schaeffer provided the impetus and was responsible for much of the early work. Dr. W. Conard Fernelius gave invaluable help as the American representative to the Inorganic Nomenclature Commission of the International Union of Pure and Applied Chemistry.

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The drawings were prepared by Mr. William Kurvach.

Appendix

The Appendix consists of Figures 1–23, which follow.

B_2H_6

FIG. 1

B_4H_{10}

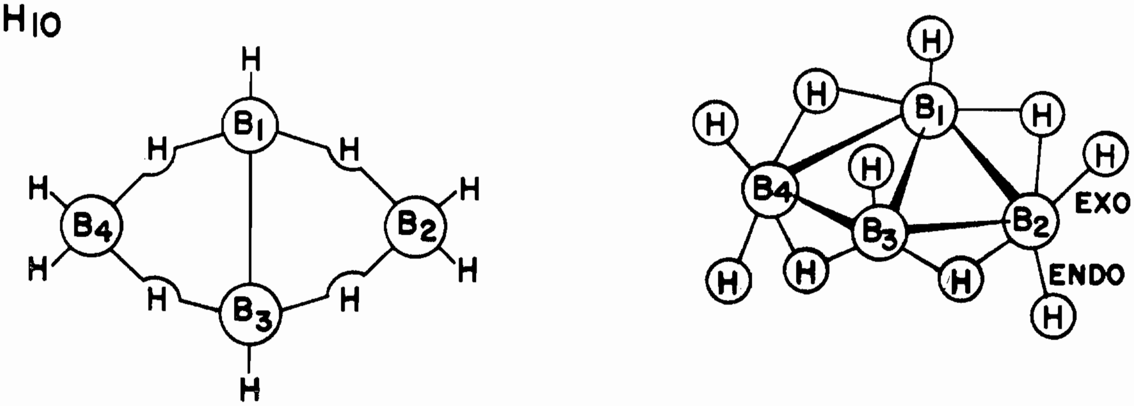


FIG. 2

endo-2,4-ethylenetetraborane(10)

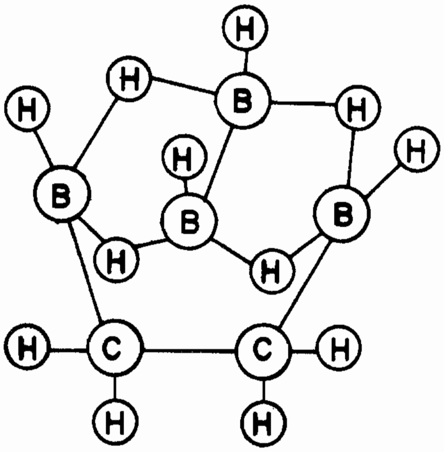


FIG. 2a

B_5H_9

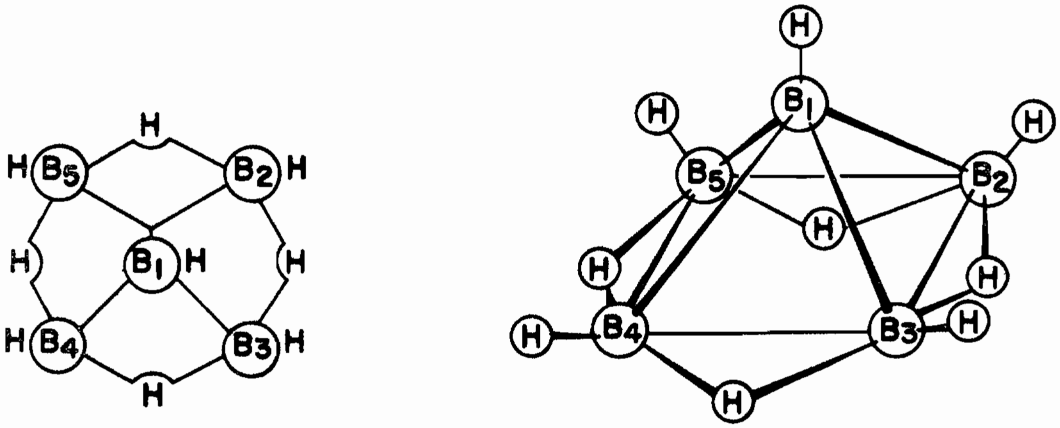


FIG. 3

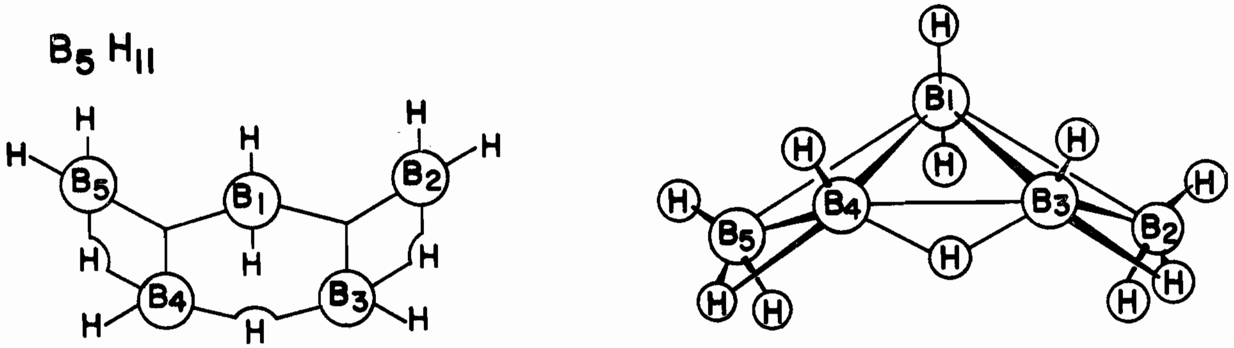


FIG. 4

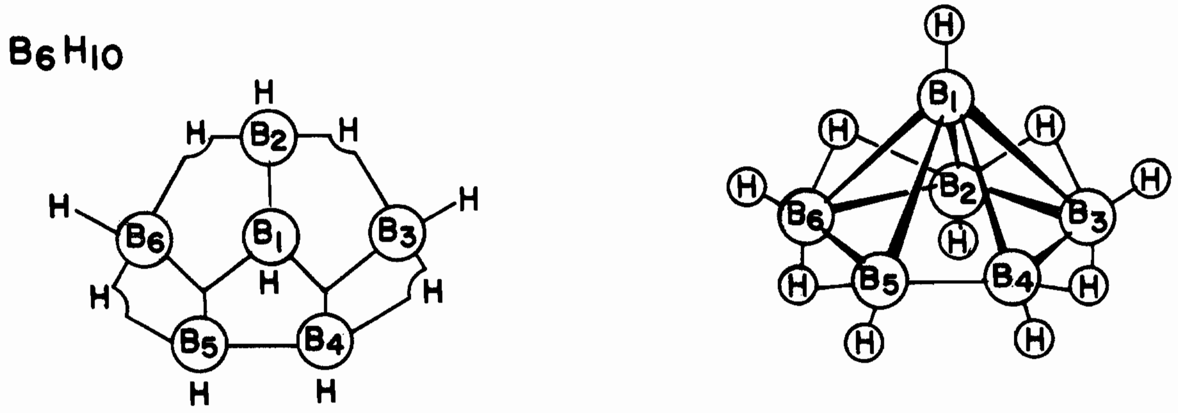


FIG. 5

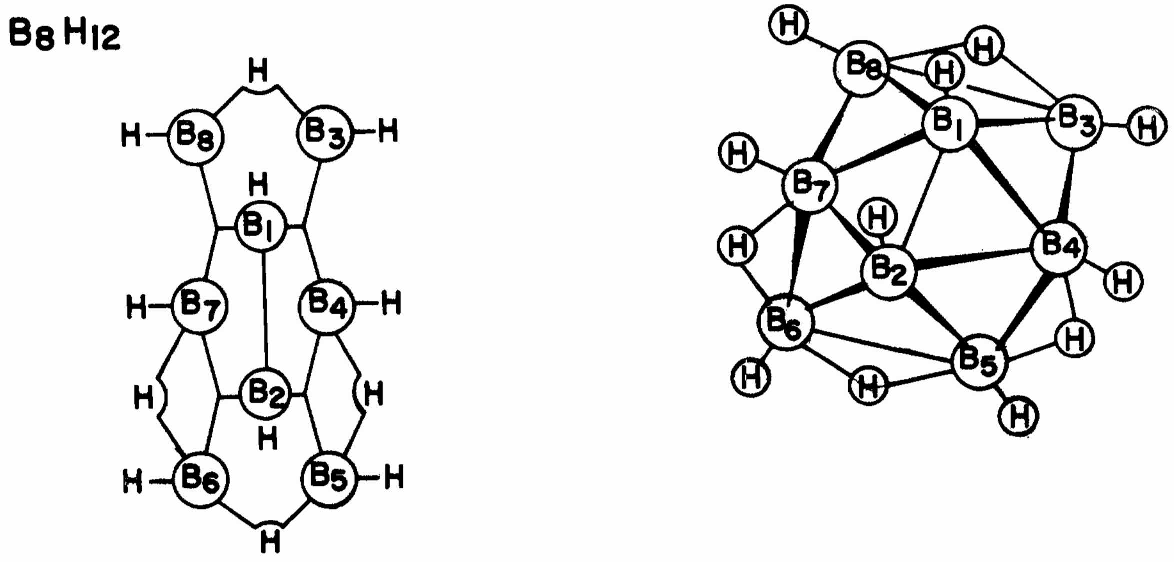


FIG. 6

B_9H_{15}

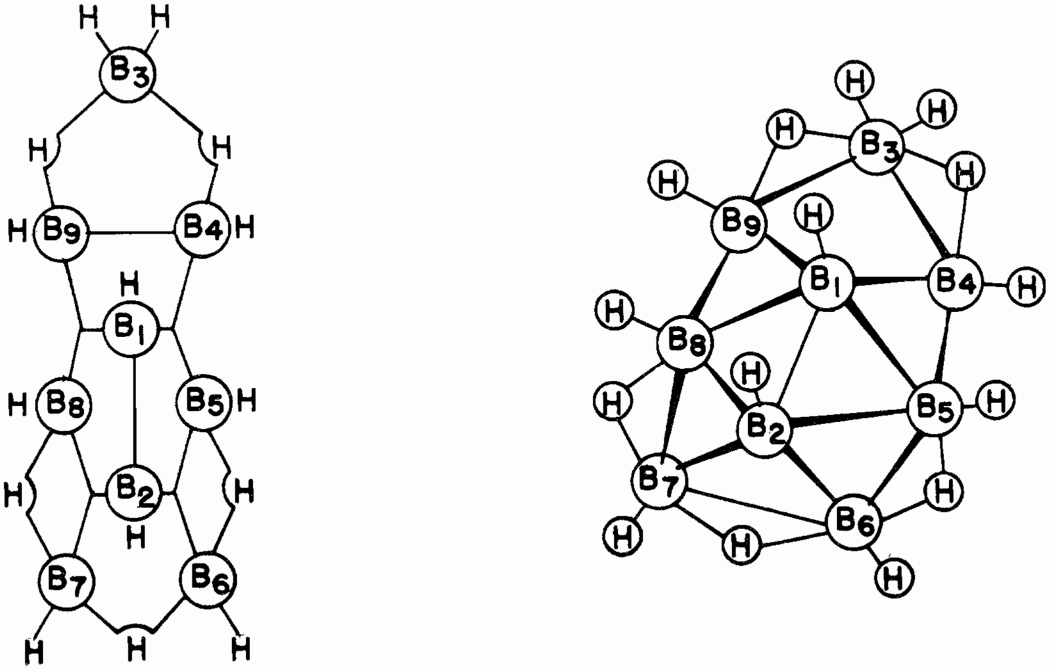
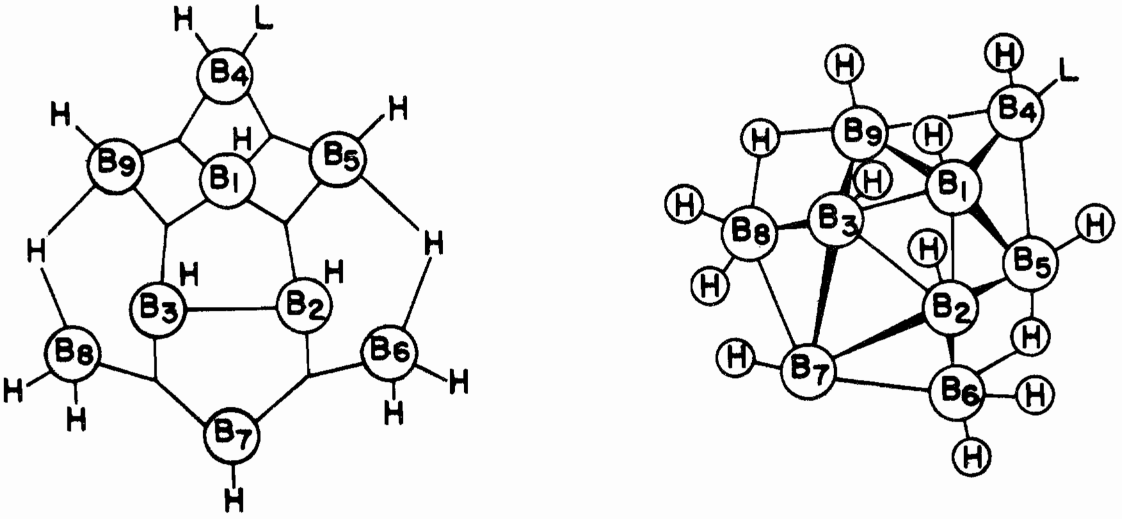


FIG. 7

$B_9H_{13}L$



L= ligand

FIG. 8

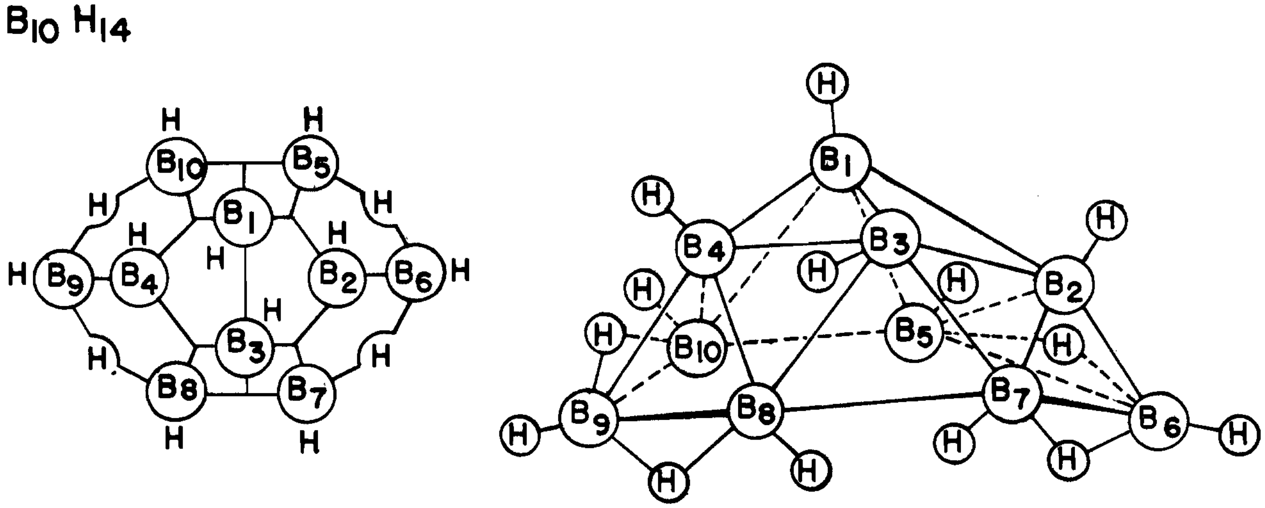

$B_{10}H_{14}$
B1
B2
B3
B4
B5
B6
B7
B8
B9
B10
H

FIG. 9

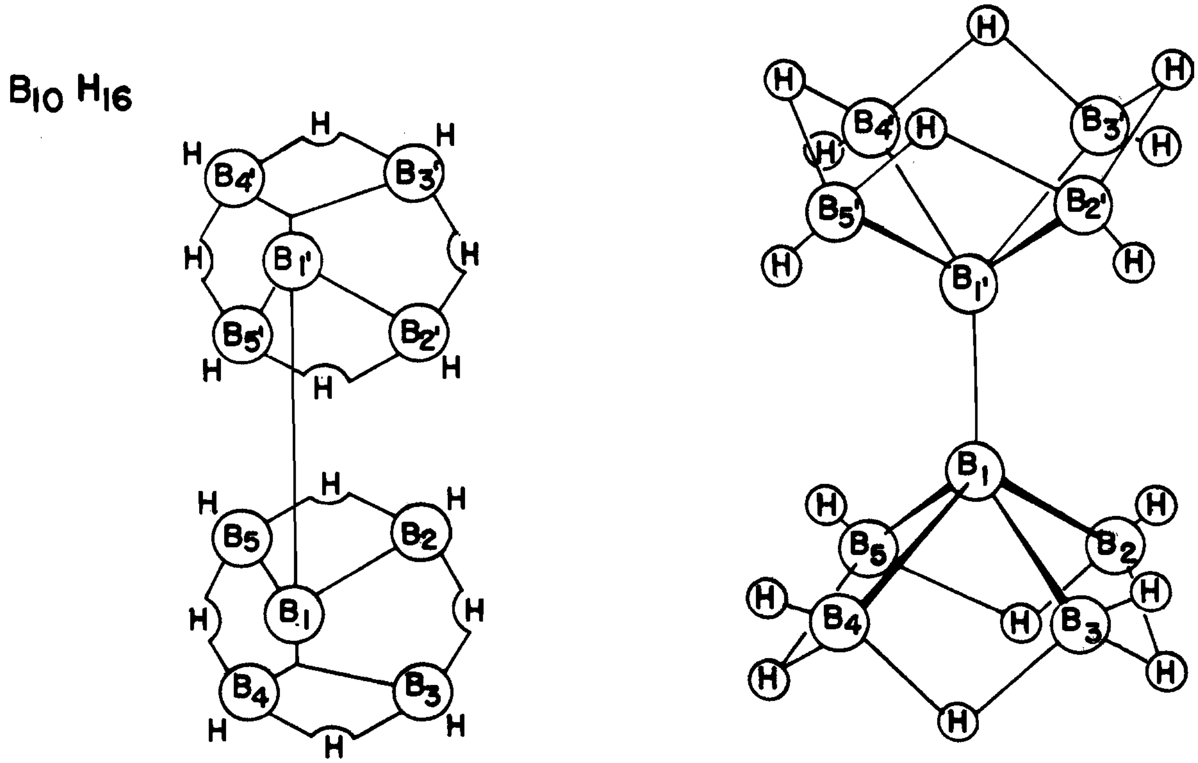
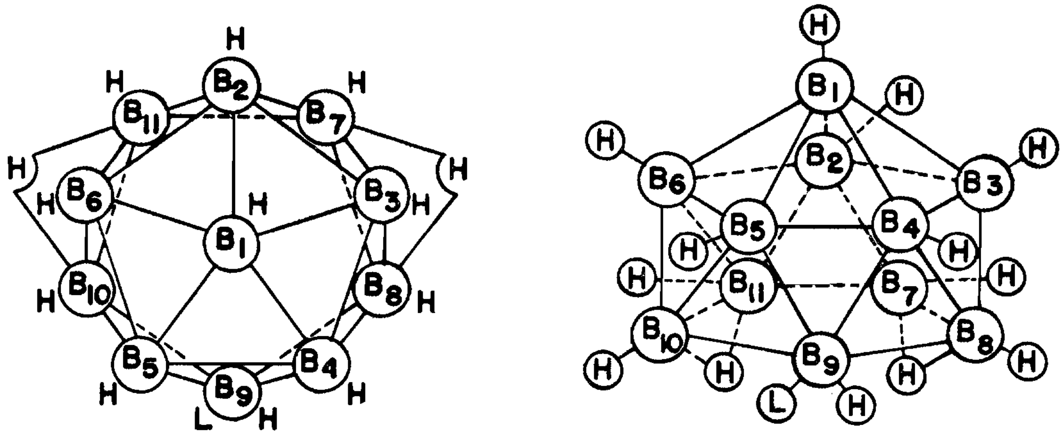

$B_{10}H_{16}$
B1'
B2'
B3'
B4'
B5'
B1
B2
B3
B4
B5
H

FIG. 10

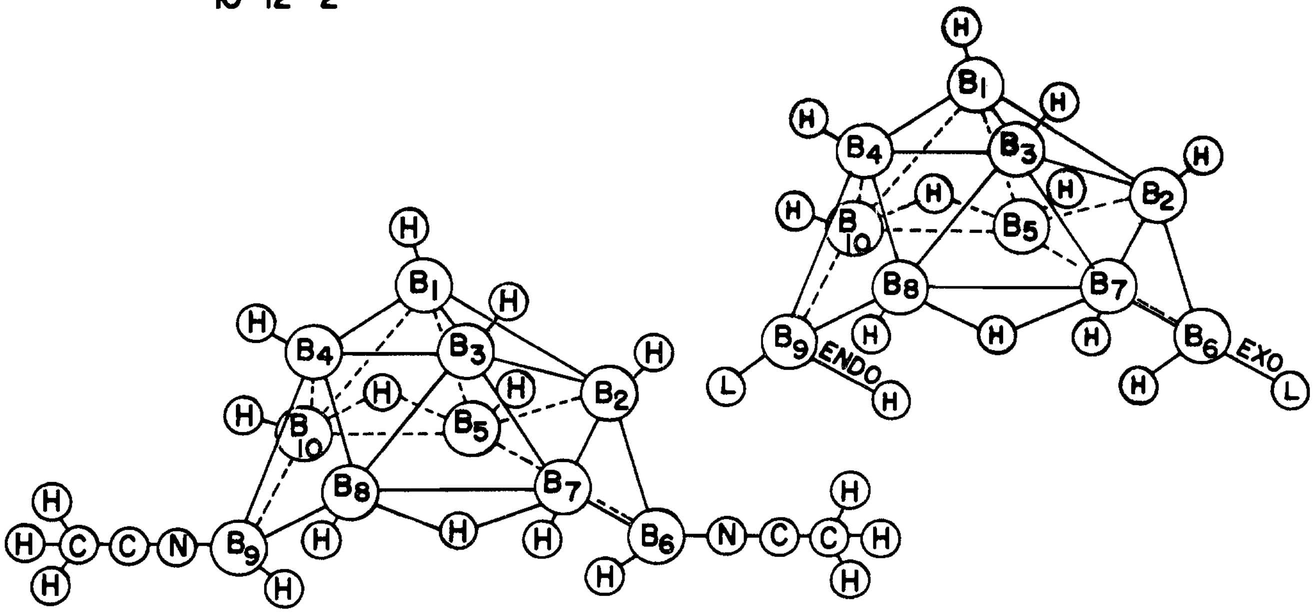
$B_{11}H_{13}L$



nido-undecaborane
with attached ligand

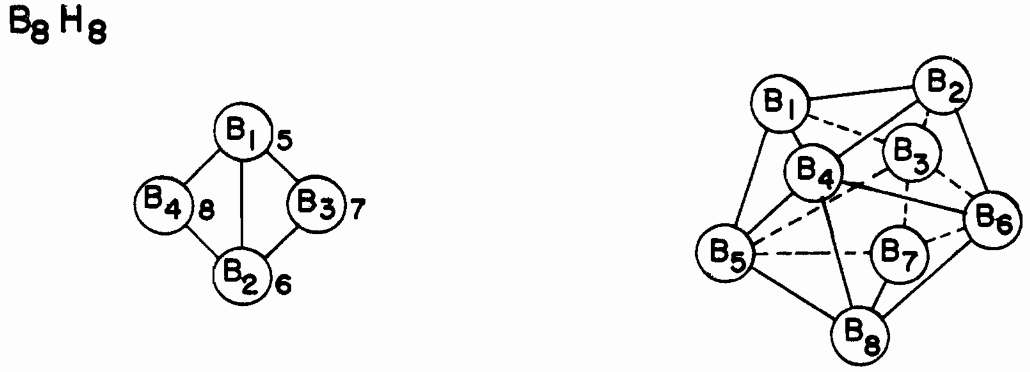
FIG. 11

$B_{10}H_{12}L_2$



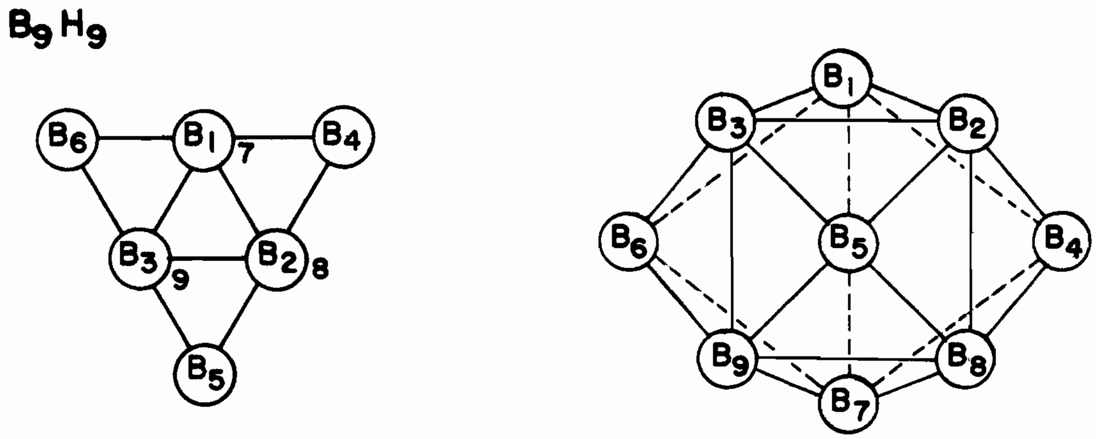
exo-bis(acetonitrile) decaborane(12)

FIG. 12



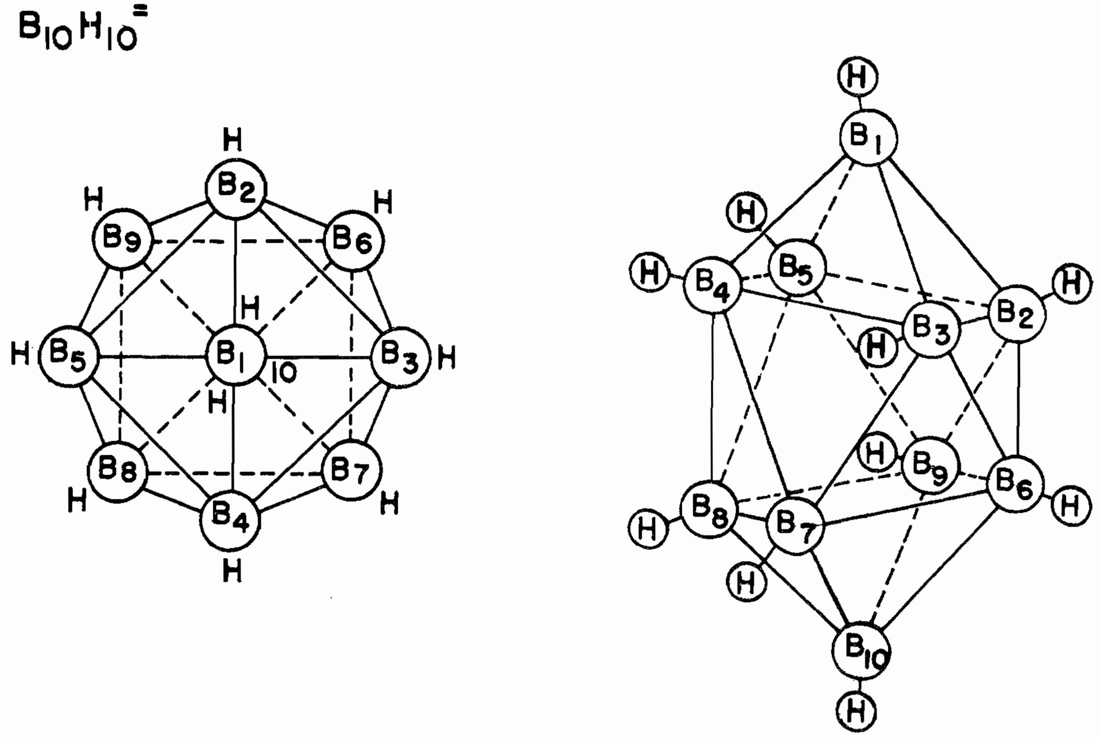
closo-octaborane(8) skeleton
(dodecahedron)

FIG. 13



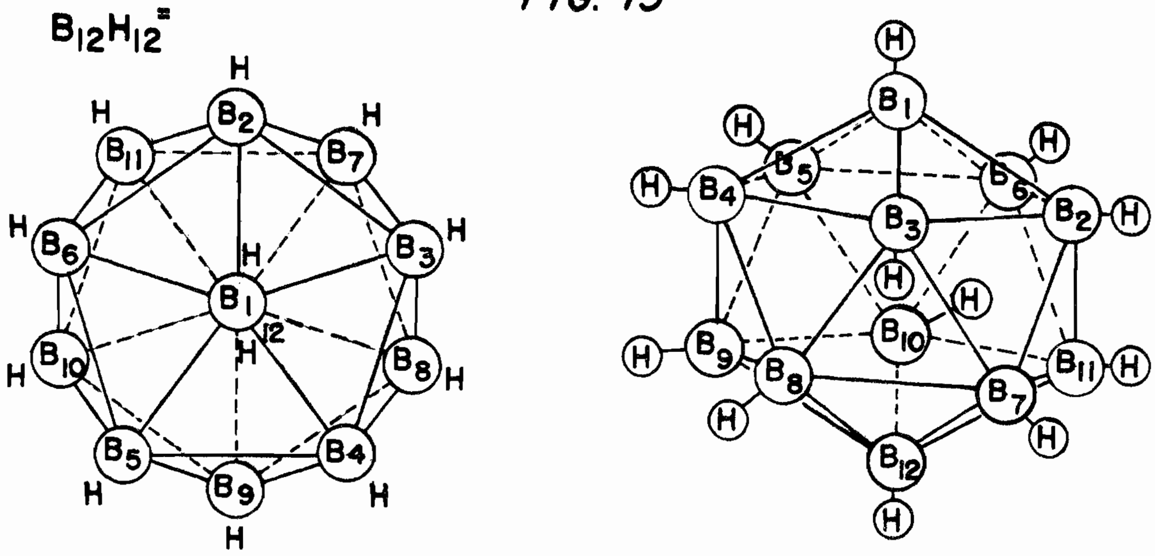
closo-nonaborane skeleton
(tricapped trigonal prism)

FIG. 14



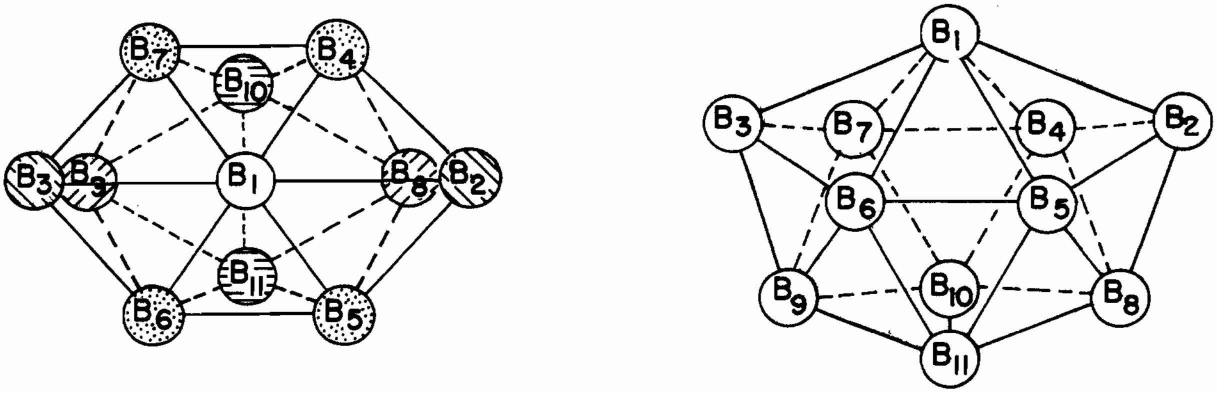
decahydro-<u>closo</u>-decaborate(2-)
(bicapped square antiprism)

FIG. 15



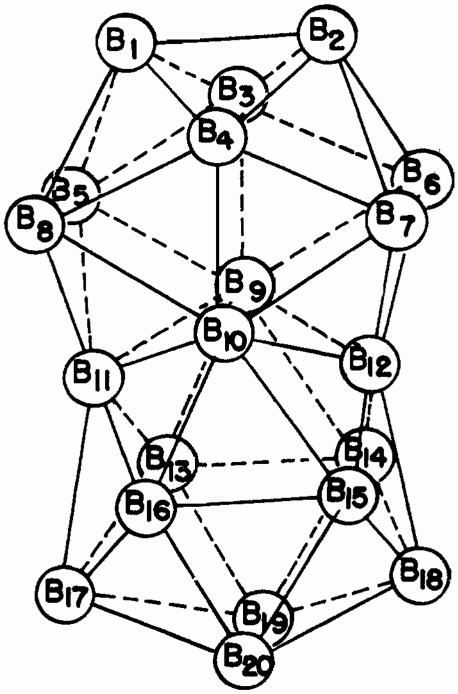
dodecahydro-<u>closo</u>-dodecaborate(2-)
(icosahedron)

FIG. 16



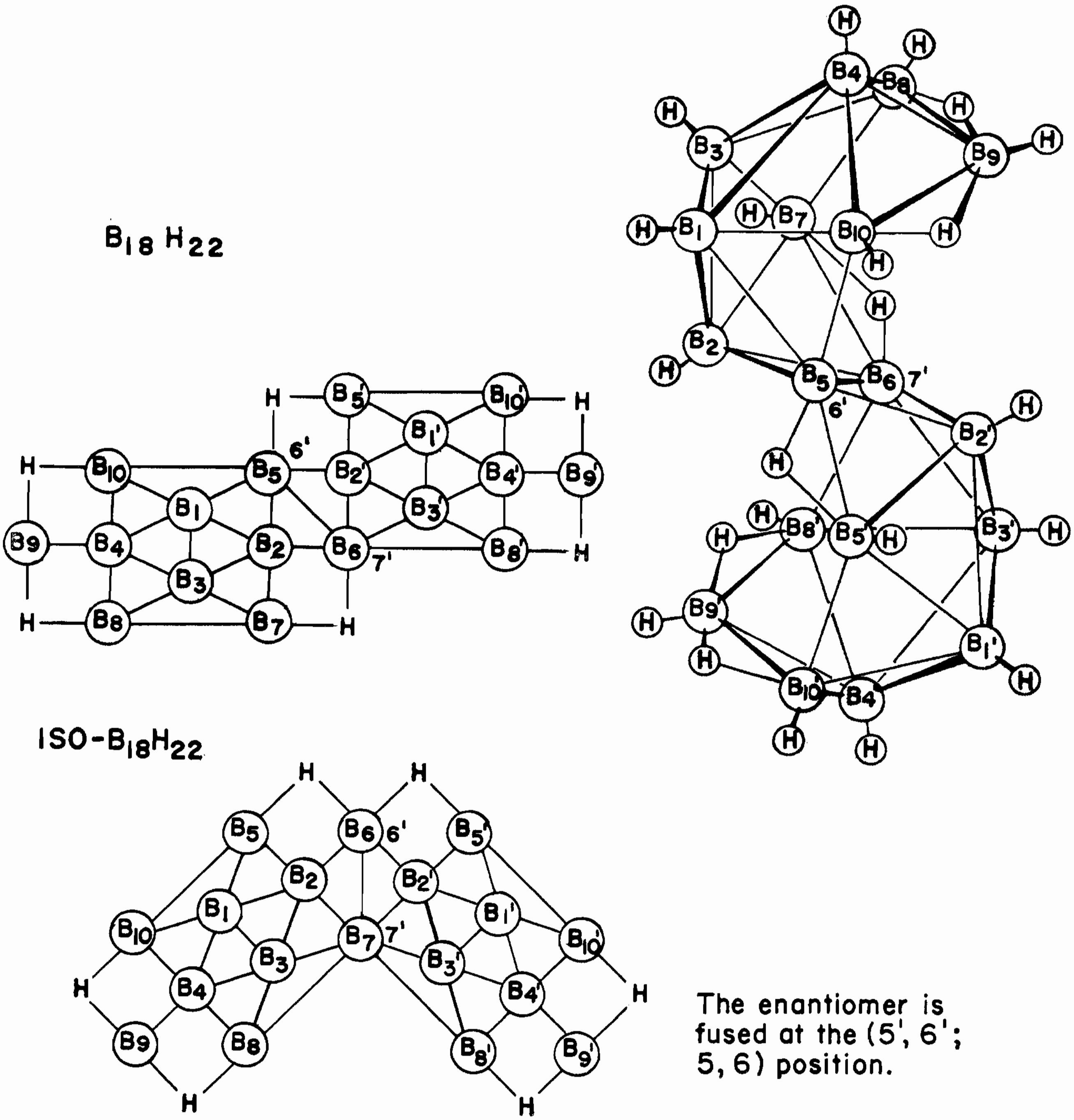
closo-undecaborane skeleton

FIG. 17



closo-icosaborane(16) skeleton

FIG. 18



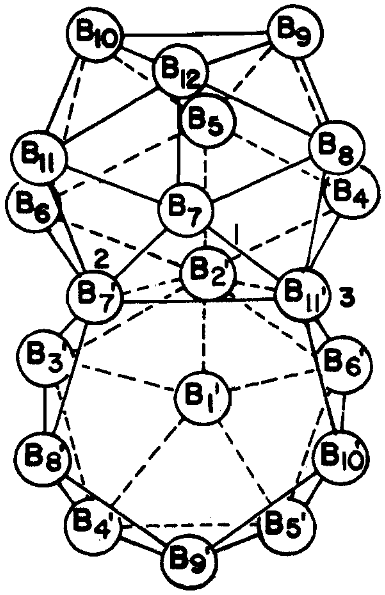
$B_{18}H_{22}$

ISO-$B_{18}H_{22}$

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

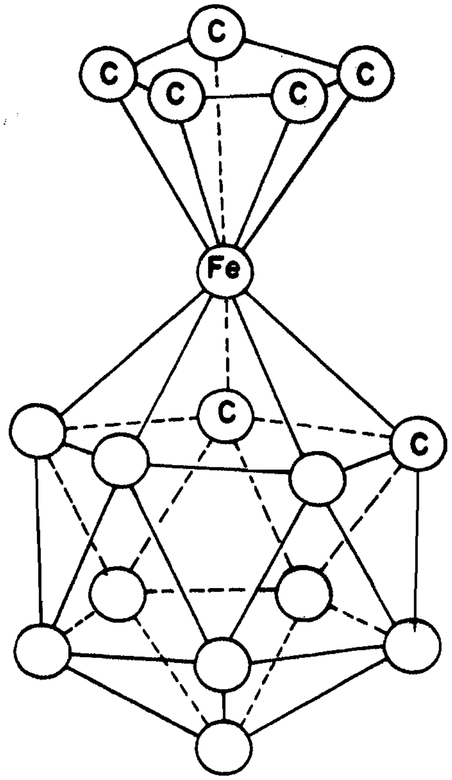
FIG. 19

$B_{20}H_{16}L_2$



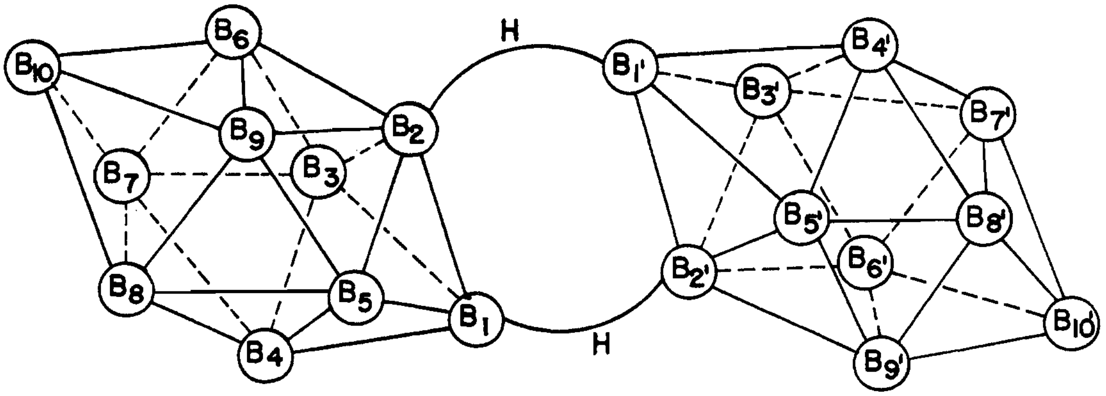
nido-undecaborano[2′, 7′, 11′: 1, 2, 3]-closo-dodecaborane skeleton

FIG. 20



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

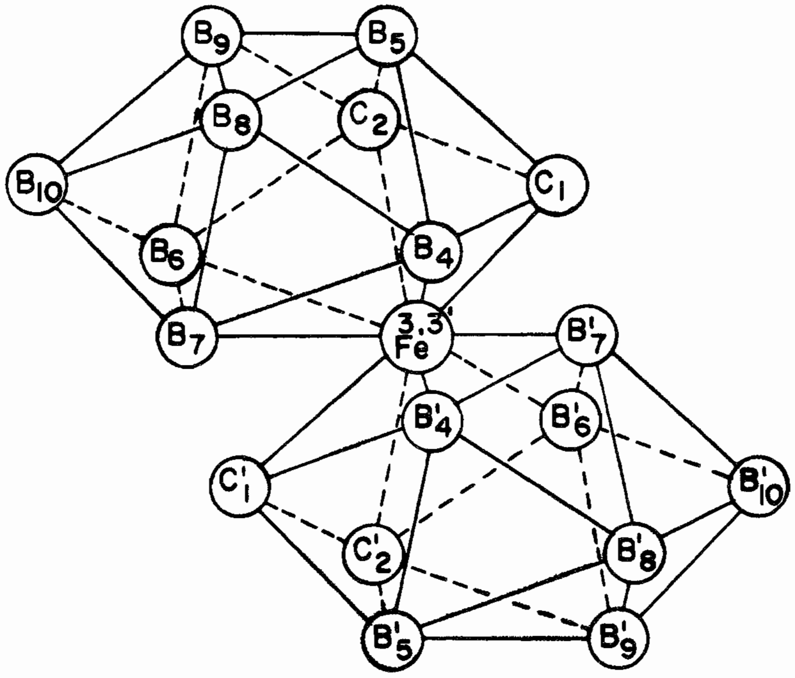
FIG. 21



1, 2′: 1′, 2-di-μ-hydro-bis[octahydro-closo-decaborate](2−)

$B_{20}H_{18}^{2-}$

FIG. 22



terminal H is omitted

3, 3'-*commo*-bis[nonahydro-1, 2-dicarba-3-
ferra-*closo*-decaborate](1-)

FIG. 23