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Structural Nomenclature for Polyboron Hydrides and Related Compounds. 3. Linear *conjuncto* Structures[1]

JAMES B. CASEY,[2a] WILLIAM J. EVANS,[2b] and WARREN H. POWELL*[2a]

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The descriptor system and methods for uniquely describing closed and nonclosed polyboron hydrides reported previously are applied to naming polyboron hydride structures consisting of two or more polyhedra or polyhedral fragments.

Introduction

One of the most complex problems in polyboron hydride nomenclature is the structural description of compounds consisting of two or more polyhedral units or polyhedral fragments. The generic term "*conjuncto*-boranes" was introduced to describe such polyboranes,[3] which in this report will be generalized by including the corresponding polyboron hydride ions and heteropolyboron hydrides. Lipscomb has discussed ten different bonding modes presently known to connect polyhedral polyboron hydride units or their fragments.[4] For this report we will group linear *conjuncto*-polyboron hydrides into five types according to whether the components (1) are connected by boron–boron bonding (including three-center bonding), (2) share one common vertex, (3) share two or more common adjacent vertices, (4) are connected by bridging hydrogen atoms, or (5) are connected by more than one of the above ways.

Only a few *conjuncto*-polyboron hydrides are treated in the current nomenclature rules,[5,6] and these are limited to compounds where the individual components are identical. Simple adaptations of organic nomenclature principles for these systems are more or less adequate. For instance, decaborane(16), consisting of two pentaborane(9) residues directly connected by a boron–boron bond, was named like a hydrocarbon ring assembly,[7a] i.e., 1,1′-bipentaborane(9).[5a,6a] Octadecaborane(22), consisting of two decaborane(14) residues that share two adjacent vertices (an edge), was named by following principles used for fused-ring systems,[7b] i.e., decaborano(14)[6′,7′:5,6]decaborane(14).[5a,6a] A technique used for naming spiro systems[7c] was adapted for naming $(B_9C_2H_{11})_2Ni$, where a nickel atom is shared between two $[I_h\text{-}(1551)\text{-}\Delta^{20}\text{-}closo]$ polyhedra, i.e., 3,3′-*commo*-bis[1,2-dicarba-3-nickela-*closo*-dodecaborane(11)].[5b] In this name, the term "commo" signified a common (metal) atom shared between the two polyhedra.

Although these techniques do suffer from certain deficiencies,[1a,b] given some modifications, as discussed below, they could be adequate for many *conjuncto*-polyboranes and some ionic *conjuncto*-polyboron hydrides. However, they are not adequate for the broad range of *conjuncto*-polyboron hydride structures known today. Lack of a method for describing more complicated *conjuncto* structures has been recognized as a major problem in boron nomenclature for over 10 years.

In this paper we propose a general scheme for naming linear *conjuncto*-polyboron hydride compounds using the descriptor method developed in our earlier papers.[1] To our knowledge, no branched *conjuncto*-polyboron hydride systems have yet been reported.[8]

General Method

Several general features of our proposal apply to the names of *conjuncto*-polyboron hydrides regardless of the manner in which the components are connected. In order to most easily visualize the structure of a *conjuncto*-compound as the name is read, we favor the following general format:[9] [a structural description of the first component]-(a locant description of attachment(s) between the first and second components)-[a structural description of the second component]-(a locant description of attachment(s) between the second and third components)-...-[the last component]-[stoichiometric name giving the total number of skeletal atoms in all components and a neutral or ionic ending](number of hydrogen atoms, if neutral; charge, if ionic).

In this report, we will call the locant description of attachment(s) between the components a "link notation". In a shortened form, the general name would look as follows: [descriptor]-(link)-[descriptor]-(link)-[descriptor]...[(numerical prefix)[10](bor)(suffix)](00). Indicated hydrogen, hydro pre-

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(1) (a) Part 1: Casey, J. B.; Evans, W. J.; Powell, W. H. *Inorg. Chem.* **1983**, *22* (16), 2228–2235. (b) Part 2: Casey, J. B.; Evans, W. J.; Powell, W. H. *Ibid.* **1983**, *22* (16), 2236–2245. (c) *Ibid.* **1981**, *20* (5), 1333–1341. (d) *Ibid.* **1981**, *20* (10), 3556–3561.

(2) (a) Chemical Abstracts Service. (b) The University of California; Camille and Henry Dreyfus Teacher-Scholar; Alfred P. Sloan Research Fellow.

(3) Boocock, S. K.; Greenwood, N. N.; Kennedy, J. D.; McDonald, W. S.; Staves, J. *J. Chem. Soc., Dalton Trans.*, **1980**, 790–796.

(4) Lipscomb, W. N. *Inorg. Chem.* **1980**, *19* (5), 1415–1416.

(5) Americal Chemical Society. "The Nomenclature of Boron Compounds", *Inorg. Chem.* **1968**, *7* (10), 1945–1964: (a) Rule 1.41, p 1947; (b) Rule 4.3, p 1951; (c) Rules 3.2–3.4, p 1950; (d) Figure 20, p 1963; (e) Figure 22, p 1963.

(6) International Union of Pure and Applied Chemistry. "Nomenclature of Inorganic Boron Compounds", *Pure Appl. Chem.* **1972**, *30* (3–4), 683–710: (a) Rule 2.31, p 686; (b) Rule 7.3, p 698; (c) Rules 4.2–4.3, 7.4, pp 690–693, 698; (d) Figure 20, p 708; (e) Figure 22, p 709.

(7) International Union of Pure and Applied Chemistry. "Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F, and H"; Pergamon Press: Oxford, 1979: (a) Rule A-52, pp 42–43; (b) Rule A-21, pp 20–25; (c) Rule A-41.5, p 39; (d) Rule A-42, pp 40–41; (e) Rule C-14.11, pp 101–105; (f) Rule E-0, p 473.

(8) The proposals herein are readily extendable to branched systems provided that criteria are developed to determine a priority order for numbering the branches. This is also a general need of nomenclature in other areas.

(9) This format may be considered to be patterned after one of the alternative methods for naming spiro compounds.[7d]

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Table I. Linking Notations for Linear *conjuncto*-Polyboron Hydride Structures

type of connection	link notation	structure
two-center boron–boron bonding	-1:2′-	1A
three-center boron–boron bonding	-2:2′,3′-	1B
one shared vertex	-1-*commo*-1′-	1C
two shared vertices (edge fused)	-2,4-*dicommo*-4′,2′-	1D
three shared vertices[a]	-1,2,3-*tricommo*-2′,7′,11′-	1E
bridging hydrogen	-1-μH-2′-	1F

[a] Face fused or a fusion of two edges having a common vertex.

fixes, substituents and ligands, heteroatom prefixes, and the prefixes "cyclo" and "seco" would be cited in the appropriate order[1a,b] in front of this basic name. This format has a number of important advantages[11] over methods based on organic principles:[5a,b,6a,b] (1) the *total* number of hydrogen atoms in a neutral polyboron hydride is given at the end of the name; (2) the *total* number of skeletal boron atoms is given by one numerical prefix; (3) the *actual* number of heteroatoms is always indicated by the appropriate prefix(es); and (4) linear combinations of polyhedral components connected in different ways can be described easily.

There are variations that could be used while still following this basic format. To include many alternatives in different cases would unnecessarily complicate our presentation. Accordingly, we discuss here only the few variations that we feel are best. We realize that other variations might be more useful under certain circumstances.

The **descriptors** we will use are the structural descriptors developed in earlier papers for closed and capped polyhedra[1a,c,d] and for nonclosed structures.[1b] The prefixes *nido* and *arachno* cannot be used in our general format because to be structurally meaningful they must refer to specific nonclosed components.

To make it easier to visualize the individual components in a *conjuncto* structure which, according to the above proposed format, has only the total number of skeletal boron atoms at the end of the name, we suggest adding a number to each separate descriptor indicating the number of vertices in that individual component. We favor placing this information in front of each descriptor as an arabic number followed by the italic letter *v* (for vertex) enclosed in parentheses, for example, $(12v)[I_h\text{-}(1551)\text{-}\Delta^{20}\text{-}closo]$.[12,13] Furthermore, we would suggest that this designation be considered an option, just as the citation of superscript numbers to the *v*'s, and the *v*'s themselves, in the description of the planes of vertices for some polyhedra as described earlier.[1c]

The **link notation** between the descriptors for the components of a *conjuncto*-structure consists of three parts: (1) the locant for the connecting vertex (or locants for the connecting vertices) of the component whose descriptor precedes the link; (2) a symbolism indicating the manner in which the two components are joined; (3) the locant for the connecting vertex (or the locants for the connecting vertices) of the component whose descriptor follows the link. Locants in the set of locants at the beginning of the link are cited in increasing numerical order, but locants in the set at the end of the link must be cited in the same order as the locants in the set at the beginning of the link to which they correspond. The various types of connections included in this report are summarized in Table I (for corresponding structures, see Figure 1).

Numbering. Each component is oriented and numbered individually, first without regard to atoms at the vertices, according to principles for numbering skeletal features of closed and capped closed polyhedra and polyhedral fragments described in earlier papers.[1] When there is a choice, components are numbered clockwise or counterclockwise so that skeletal positions attached to or in common with the next component are as low as possible.[14] Thus, the skeletal structure given by the descriptor for a *conjuncto* system is numbered as fully as possible before numbering heteroatoms and other skeletal features described by prefixes appearing in front of the descriptor.

If there is a choice for numbering individual components, preference for low locants is given to heteroatoms first as a complete set, regardless of the nature of the heteroatom, and then to the heteroatoms in their order of seniority, i.e., in their order of appearance in the list of replacement prefixes given in Table I in part 1 of this series.[1a]

Locants of the different components are distinguished by primes. Unprimed locants are given to the preferred terminal component determined as described below. The component attached to the preferred terminal component is assigned primed locants; locants of successive components are primed serially.

The preferred terminal component has the largest number of vertices actually present. When both terminal components have the same number of vertices, we suggest that a closed polyhedron be preferred over a nonclosed structure. For two

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(10) Numerical prefixes beyond 20 are much less common than those below 20. Hence, for convenience, we illustrate here the formation of names for numerical prefixes above 20:

20	icosa	30	triaconta	40	tetraconta
21	henicosa	31	hentriaconta	50	pentaconta
22	docosa	32	dotriaconta	60	hexaconta
23	tricosa	33	tritriaconta	70	heptaconta
24	tetracosa	34	tetratriaconta	80	octaconta
	etc.		etc.	90	nonaconta
				100	hecta

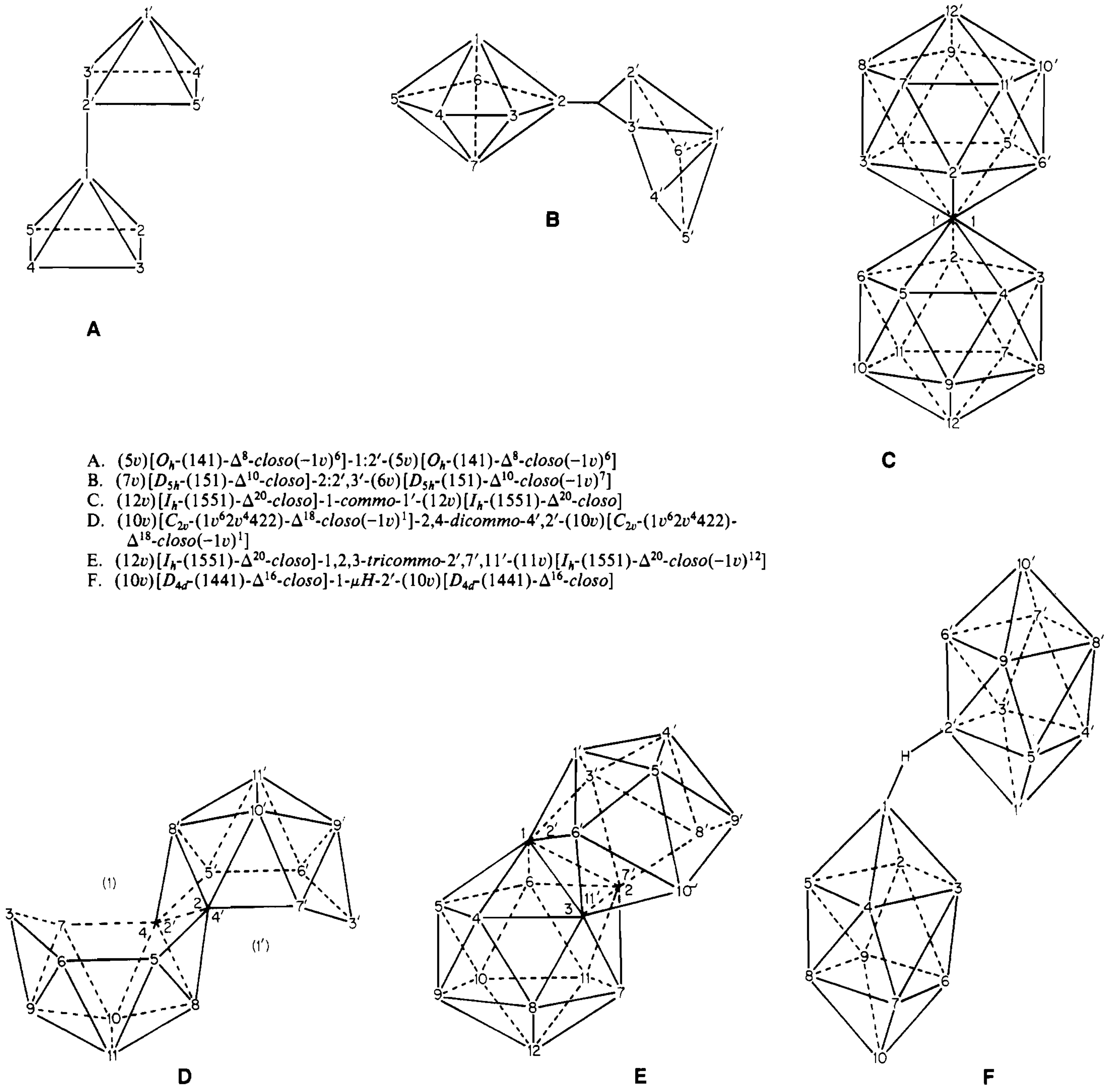
Although numerical prefixes are preferred in systematic chemical nomenclature, arabic numerals have been used occassionally, for example, in describing addition compounds. See: International Union of Pure and Applied Chemistry. "Nomenclature of Inorganic Chemistry (1970)", 2nd ed.; Butterworths: London, 1971; pp 8, 84.

(11) The disadvantage of methods in the current rules can be illustrated as follows: From the names 1,1′-bipentaborane(9) and decaborano(14)-[6′,7′:5,6]decaborane(14), it could be inferred that the respective compounds had 18 and 28 hydrogen atoms, when in fact the number of hydrogen atoms is 16 and 22, respectively. The name 3,3′-*commo*-bis[1,2-dicarba-3-nickela-*closo*-dodecaborane(11)] implies a total of 24 skeletal atoms, 2 of which are nickel atoms, when in fact there are 23 skeletal atoms and only 1 nickel atom. Although such concerns are relatively unimportant in organic nomenclature, from which the methods for naming these boron compounds were derived, they are crucial to understanding the nomenclature of boron compounds because, as we discussed before,[1a,b] names for boron compounds explicitly express the number of hydrogen atoms and skeletal atoms.

(12) Other formats are possible. However, to use this technique for capped closed and nonclosed components as well as for closed ones, this notation must be outside the brackets that define the complete descriptor. We feel that it is also important for this notation to precede the descriptor so that the entire descriptor allows the structure to be revealed in a natural sequence; for example, a $(8v)[D_{5h}\text{-}(1v^5 5v^4 1v^5)\text{-}\Delta^{10}\text{-}closo\text{-}(+1v)^{1,2,3}]$ polyhedron is an "eight-vertex D_{5h} polyhedron having three parallel planes of vertices, the first plane having one vertex with five skeletal connections, the second plane containing five vertices each with four skeletal connections, and the third plane having one vertex with five skeletal connections; the polyhedron has ten triangulated faces, and is capped by one vertex located on the face defined by the vertex locants 1, 2, and 3". A superscript format is possible, but it seems to us to be less desirable.

(13) An alternative format applicable to multi(polyhedral) systems only would be to cite the vertices of each individual component ahead of the general descriptor given above, for example, (10*v*,12*v*,6*v*)-[descriptor]-link-[descriptor]....

(14) Nonterminal components are numbered so that the skeletal positions attached to or in common with both other components are as low as possible, first as a set and then in order of citation in the link; for example, in Figure 4 1,7 is preferred to 2,4 and in Figure E in the supplementary material 1,7,1,7 is preferred to 1,7,7,1.



A. $(5v)[O_h\text{-}(141)\text{-}\Delta^{8}\text{-}closo(-1v)^{6}]\text{-}1{:}2'\text{-}(5v)[O_h\text{-}(141)\text{-}\Delta^{8}\text{-}closo(-1v)^{6}]$
B. $(7v)[D_{5h}\text{-}(151)\text{-}\Delta^{10}\text{-}closo]\text{-}2{:}2',3'\text{-}(6v)[D_{5h}\text{-}(151)\text{-}\Delta^{10}\text{-}closo(-1v)^{7}]$
C. $(12v)[I_h\text{-}(1551)\text{-}\Delta^{20}\text{-}closo]\text{-}1\text{-}commo\text{-}1'\text{-}(12v)[I_h\text{-}(1551)\text{-}\Delta^{20}\text{-}closo]$
D. $(10v)[C_{2v}\text{-}(1v^{6}2v^{4}422)\text{-}\Delta^{18}\text{-}closo(-1v)^{1}]\text{-}2,4\text{-}dicommo\text{-}4',2'\text{-}(10v)[C_{2v}\text{-}(1v^{6}2v^{4}422)\text{-}\Delta^{18}\text{-}closo(-1v)^{1}]$
E. $(12v)[I_h\text{-}(1551)\text{-}\Delta^{20}\text{-}closo]\text{-}1,2,3\text{-}tricommo\text{-}2',7',11'\text{-}(11v)[I_h\text{-}(1551)\text{-}\Delta^{20}\text{-}closo(-1v)^{12}]$
F. $(10v)[D_{4d}\text{-}(1441)\text{-}\Delta^{16}\text{-}closo]\text{-}1\text{-}\mu H\text{-}2'\text{-}(10v)[D_{4d}\text{-}(1441)\text{-}\Delta^{16}\text{-}closo]$

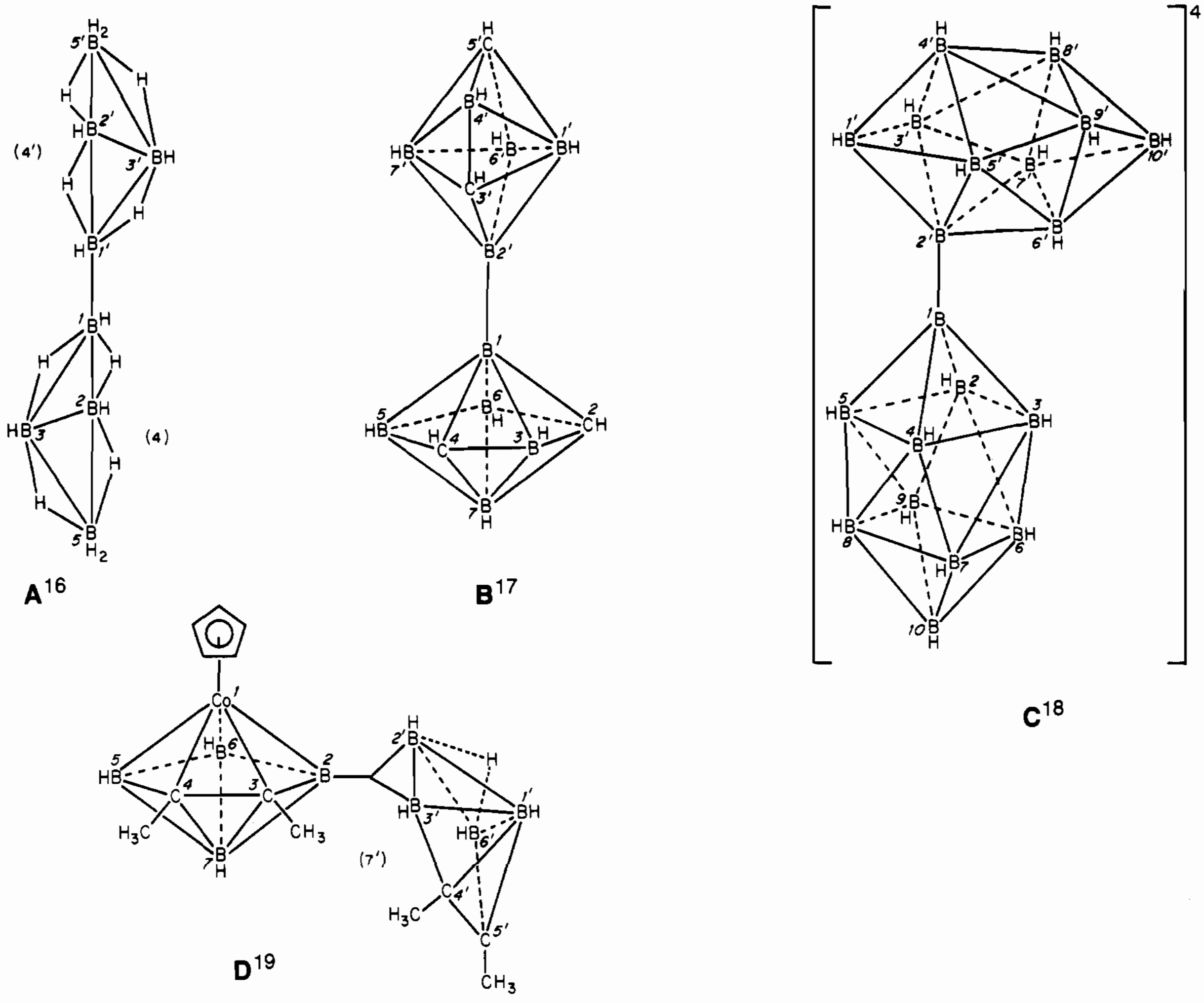
Figure 1. *conjuncto*-Polyboron hydride descriptors.

terminal nonclosed structures, we suggest that the preferred polyhedral fragment have the fewer missing vertices determined by comparing with the closed polyhedron from which it is derived. Further criteria, which we will not detail here, could follow principles for choosing a senior organic ring system.[7c] Two of these criteria, namely, the greater number of heteroatoms and lower locants for heteroatoms, are illustrated by examples in Figures C and D in the supplementary material.

Examples of descriptor assemblies for the two-component *conjuncto* systems of Table I are shown in Figure 1.

Names for Specific *conjuncto*-Polyboron Hydrides and Related Compounds

The generation of names for *conjuncto*-polyboron compounds whose components are connected by one of the six types of linkages given in Table I and illustrated in Figure 1 is treated in the next four sections of this report, followed by a discussion of structures having more than one general type of connection between two components. Principles for treating neutral and ionic polyboron hydrides, their hetero analogues, and derivatives established in two previous papers[1a,b] are used in naming specific compounds as illustrated in the sections that follow. In *conjuncto* systems we will assume that the vertices connecting two polyhedra or polyhedral fragments have no hydrogen atoms attached to them; this is by far the most common situation. Hence, the previously discussed principle[1a,b] that one and only one hydrogen atom is attached to each carbon and boron skeletal atom is modified in *conjuncto* compounds in that it applies to all vertices except those joined to or shared with other components. If there are hydrogen atoms at linking or shared vertices, they must be specified by one of the techniques described earlier,[1a,b] just as extra hydrogen atoms on boron and carbon atoms at other vertices,



A. 1*H*,1′*H*,5*H*,5′*H*-(1,2-μ*H*),(1′,2′-μ*H*),(1,3-μ*H*),1′,3′-μ*H*),(2,5-μ*H*),(2′,5′-μ*H*),(3,5-μ*H*),(3′,5′-μ*H*)[(4*v*)[D_{3h}-(131)-Δ^6-*closo*(−1*v*)^4]-1:1′-(4*v*)[D_{3h}-(131)-Δ^6-*closo*(−1*v*)^4]octaborane](18)[20a]

B. 2,3′,4,5′-tetracarba[(7*v*)[D_{5h}-(151)-Δ^{10}-*closo*]-1:2′-(7*v*)[D_{5h}-(151)-Δ^{10}-*closo*]tetradecaborane](12)

C. octadecahydro[(10*v*)[D_{4d}-(1441)-Δ^{16}-*closo*]-1:2′-(10*v*)[D_{4d}-(1441)-Δ^{16}-*closo*]icosaborate](4−)

D. 1-(η^5-cyclopentadienyl)-3,4,4′,5′-tetramethyl-2′*H*,3′*H*-(2′,6′-μ*H*)[1-cobalta-3,4,4′,5′-tetracarba[(7*v*)[D_{5h}-(151)-Δ^{10}-*closo*]-2:2′,3′-(6*v*)[D_{5h}-(151)-Δ^{10}-*closo*(−1*v*)^7]tridecaborane]](12)[20b]

Figure 2. *conjuncto*-Polyboron hydrides connected by boron–boron bonding.

bridging hydrogen atoms, and all hydrogen atoms on skeletal atoms other than boron and carbon atoms must be specified.

The generality and structural explicitness of the "linking descriptor" method we propose is obvious. However, in certain cases, primarily those with symmetrical structures, simpler names are possible by extending and modifying the techniques used in the current rules,[5a,b,6a,b] particularly where the use of the prefixes *nido* or *arachno* is possible. Therefore, when applicable in subsequent sections, after giving our recommended method, we will discuss methods based on techniques given in the current rules modified to accomodate the following suggestions: (1) the prefixes *nido* and *arachno* are used only when a nonclosed polyboron hydride component meets the structural and electronic criteria suggested previously;[1b] (2) the assumptions about the presence or absence of hydrogen atoms discussed in this paper and previously[1a,b] are observed; (3) "extra" and bridging hydrogen atoms in a polyborane are given by the "indicated hydrogen" method discussed earlier;[1a,b] and (4) the actual number of hydrogen atoms in a *conjuncto*-polyborane is cited as a parenthetical number at the very end of the name.[15] In addition, in order to provide the maximum generality, we suggest that as far as possible the notation of indicated hydrogen, heteroatom prefixes, and hydro ligand prefixes not be included with the name of each component as in the current rules,[5a,b,6a,b] but be cited in front of

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(15) In the current rules,[5a,b,6a,b] the number of hydrogen atoms in a component only is cited, for example, 1,2′-bipentaborane(9).[5a,6a]

(16) Rietz, R. R.; Schaeffer, R.; Sneddon, L. G. *Inorg. Chem.* **1972**, *11* (6), 1242–1244. Steck, S. J.; Pressley, G. A., Jr.; Stafford, F. E.; Dobson, J.; Schaeffer, R. *Inorg. Chem.* **1969**, *8* (4), 830–836. Dobson, J.; Gaines, D.; Schaeffer, R. *J. Am. Chem. Soc.* **1965**, *87* (18), 4072–4074.

(17) Astheimer, R. J.; Plotkin, J. S.; Sneddon, L. G. *J. Chem. Soc., Chem. Commun.* **1979**, 1108–1109.

(18) Hawthorne, M. F.; Piling, R. L.; Stokely, P. F. *J. Am. Chem. Soc.* **1965**, *87* (9), 1893–1899. Chamberland, B. L.; Muetterties, E. L. *Inorg. Chem.* **1964**, *3* (10), 1450–1456.

(19) Borelli, A. J., Jr.; Plotkin, J. S.; Sneddon, L. G. *Inorg. Chem.* **1982**, *21* (4), 1328–1331.

(20) Using the alternate method of expressing "extra" hydrogen and bridging hydrogen atoms at the end of the name: (a) [(4*v*)[D_{3h}-(131)-Δ^6-*closo*(−1*v*)^4]-1:1′-(4*v*)[D_{3h}-(131)-Δ^6-*closo*(−1*v*)^4]octaborane](18)-1,1′,5,5′-H_4-1,2:1′,2′:1,3:1′,3′:2′,5′:3′,5′-μH_8; (b) 1-(η^5-cyclopentadienyl)-3,4,4′,5′-tetramethyl[1-cobalta-3,4,4′,5′-tetracarba-[(7*v*)[D_{5h}-(151)-Δ^{10}-*closo*]-2:2′,3′-(6*v*)[D_{5h}-(151)-Δ^{10}-*closo*(−1*v*)^7]-tridecaborane](12)-2′,3′-H_2-2′,6′-μ*H*].

any numerical prefixes and brackets defining the identical components. By such a method, these features of a compound need not be symmetrically located on the separate components.

conjuncto-Polyboron Hydrides with Components Connected by Boron–Boron Bonding (Structures A and B in Figure 1)

Recommended Linking Descriptor Method. The *link notation* for this type of *conjuncto*-polyboron hydride, "locant:locant", as shown in Table I, describes the vertices of each component involved in the connection without specifically indicating the type of bonding. A three-center bond would be described by a link notation such as 2:2′,3′. Examples of *conjuncto*-polyboron hydrides with direct boron–boron bonding are given in Figure 2 and in Figures A and B of the supplementary material.

Assembly Method. An adaptation of the nomenclature principles for naming ring assemblies[7a] was used in the current rules for naming *conjuncto*-polyboranes consisting of two identical polyborane components.[5a,6a] In addition to the modifications suggested above, we would also suggest that a colon be used between the pair of locants; thus locants of the respective components are separated in the same way as suggested in our recommended method. Thus, as semisystematic names we would suggest 1:2′-bi[*nido*-pentaborane](16)[15] for (*nido*-B_5H_8)-1:2′-(*nido*-B_5H_8), whose skeletal structure is shown as A in Figure 1, and 2*H*,2′*H*-2:2′-bi[*arachno*-tetraborane](18) for the polyborane shown as A in Figure 2. Note, however, the use of "arachno" numbering[1b] for the latter name. For the compound [(*nido*-9,10-$C_2B_9H_{10}$)-7,8:7′,8′-(*nido*-9,10-$C_2B_9H_{10}$](2−),[21] we would suggest the name 7,7′-dihydrooctadecahydro[9,9′,10,10′-tetracarba-7,8:7′,8′-bi[*nido*-undecaborate]](2−).[22]

Compounds consisting of identical closed polyhedral structures or nonclosed structures for which *nido* or *arachno* prefixes cannot be used can also be described by using descriptors.[1] For example, compounds B and C in Figure 2 can be named 2,3′,4,5′-tetracarba-1:2′-bi[(7*v*)[D_{5h}-(151)-Δ^{10}-*closo*]heptaborane](12) and octadecahydro-1:2′-bi[(10*v*)[D_{4d}-(1441)-Δ^{16}-*closo*]decaborate](4−), respectively.[23]

Unsymmetrical compounds can be accomodated in this assembly method only by using the "debor" system,[1b] provided that each component can be derived from the same polyhedron. For example, compound D in Figure 2 could be named 1-(η^5-cyclopentadienyl)-3,4,4′,5′-tetramethyl-2′*H*,3′*H*-(2′,6′-μH)[1-cobalta-3,4,4′,5′-tetracarba-7′-debor-2:2′,3′-bi-[(7*v*)[D_{5h}-(151)-Δ^{10}-*closo*]heptaborane]](12).

Three component systems can also be described by the assembly method using the multiplying term "ter" and separating the preceding locant sets by a solidus or a semicolon or by enclosing each set in parentheses, so that the order of the components is clear. Thus, the compound ($C_2B_3H_4$)-2:2′-($C_2B_3H_3$)-3′:2″-($C_2B_3H_4$) (structure III in Figure A of the supplementary material) could be named 1,1′,1″,5,5′,5″-hexacarba-(2:2′)(3′:2″)-ter[(5*v*)[D_{3h}-(131)-Δ^6-*closo*]pentaborane](11).

Substitutive Method. *conjuncto*-Polyboranes can also be named by substitutive principles. One component is chosen as the parent and the other component is cited as a substitutive prefix formed according to the current rules.[5c,6c] To illustrate, such a substitutive name for compound A in Figure 2 would be 2-(*arachno*-tetraboran(10)-2-yl)-*arachno*-tetraborane(10). This type of name is more useful for unsymmetrical structures; for example, the compound (*closo*-1,6-$C_2B_4H_5$)-2:1′-(*closo*-1,5-$C_2B_3H_4$)[24] would be named 2-[1,5-dicarba(5*v*)[D_{3h}-(131)-Δ^6-*closo*]pentaboran(5)-1-yl]-1,6-dicarba(6*v*)[O_h-(141)-Δ^8-*closo*]hexaborane(6).

conjuncto-Polyboranes whose components are connected by three-center bonding can be named by substitutive principles if one component can be considered to substitute, or be substituted by, a bridging hydrogen atom of the other component. For example, compound D in Figure 2 could be named as follows: 1-(η^5-cyclopentadienyl)-4-[2,3-dimethyl-(4′,5′-μH),(5′,6′-μH)-2,3-dicarba-*nido*-hexaboran(8)-(4′,5′-μH)-yl]-2,3-dimethyl-1-cobalta-2,3-dicarba(7*v*)[D_{5h}-(151)-Δ^{10}-*closo*]heptaborane(6). Note that the numbering given in this name is not the same as shown for compound D in Figure 2; each component is numbered independently of the connecting positions.

However, some known polyboranes do not fit easily into the substitutive method (compound IV in Figure B of the supplementary material is an example), and ionic compounds would require yet another combination of substitutive and coordination principles,[1a,b] which just does not seem necessary. Thus, although perhaps more familiar, the substitutive method offers no advantage over our recommended method. The latter is completely general, is better for visualizing structure, and is completely structurally specific.

conjuncto-Polyboron Hydrides with Components Sharing One Common Atom (Structure C in Figure 1)

Recommended Linking Descriptor Method. The *link notation* for *conjuncto*-polyboron hydrides whose components are connected by only one common atom, "locant-*commo*-locant", as shown in Table I, is obviously based on the term "commo" introduced in the current rules of boron nomenclature to indicate a (metal) atom common to two polyhedral structures.[5b,6b] This term was used rather than "spiro", the term for describing organic ring systems with a common atom.[7c]

Examples of "monocommo" *conjuncto*-polyboron hydrides, i.e., structures with one common vertex between two polyhedra or polyhedral fragments, are given in Figure 3 and in Figures C and D of the supplementary material. Compound C in Figure 3 illustrates the first criterion mentioned above for choosing the component to be cited first in the descriptor, i.e., the larger number of vertices. Additional criteria are illustrated by compounds II and III in Figure C and I in Figure D in the supplementary material. Compound D in Figure 3 illustrates a "slipped sandwich" structure. Note that although we have classified these structures as "monocommo", the numerical prefix "mono" is not used in the linking notation; this is consistent with usual nomenclature practice.

"Poly(monocommo)" *conjuncto*-polyboron hydrides, i.e., structures with more than two component polyhedra or polyhedral fragments each connected to another component

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(21) Janoušek, Z.; Heřmånek, S.; Plešek, J.; Štíbr, B. *Collect Czech. Chem. Commun.* **1974**, *39* (9), 2363–2373.

(22) In this name we have given locants to the hydro ligands only where hydrogen is not assumed to be present. Obviously, this suggestion shortens the name considerably from that in which all locants for hydro ligands are specified, as was done previously[1b] and which is the usual practice.

(23) One could even remove the "bi" term by using a subscript 2 after the descriptor and include the linking locants within the descriptor; accordingly, these names would become 2,3′,4,5′-tetracarba-1:2′-[(7*v*)[D_{5h}-(151)-Δ^{10}-*closo*]$_2$tetradecaborane](12) and octadecahydro-1:2′-[(10*v*)[D_{4d}-(1441)-Δ^{16}-*closo*]$_2$icosaborate](4−), respectively.

(24) Plotkin, J. S.; Astheimer, R. J.; Sneddon, L. G. *J. Am. Chem. Soc.* **1979**, *101* (15), 4155–4163.

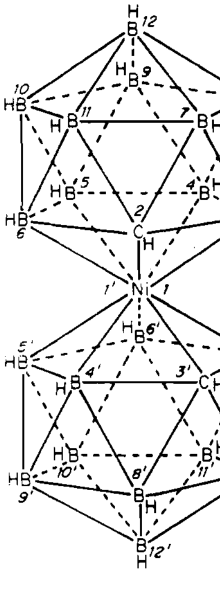
(25) Warren, L. F., Jr.; Hawthorne, M. F. *J. Am. Chem. Soc.* **1970**, *92* (5), 1157–1173. St. Clair, D.; Zalkin, A.; Templeton, D. H. *J. Am. Chem. Soc.* **1970**, *92* (5), 1173–1179.

(26) Fronczek, F. R.; Halstead, G. W.; Raymond, K. N. *J. Am. Chem. Soc* **1977**, *99* (6), 1769–1775.

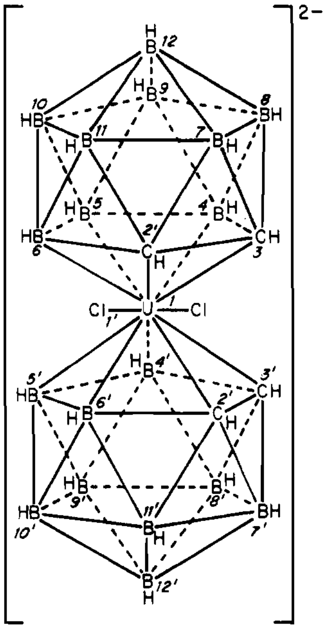
(27) (a) Churchill, M. R.; Gold, K. *Inorg. Chem.* **1973**, *12* (5), 1157–1165. (b) *J. Chem. Soc., Chem. Commun.* **1972**, 901–902.

(28) Wing, R. M. *J. Am. Chem. Soc.* **1968**, *90* (18), 4828–4834; **1967**, *89* (22), 5599–5604.

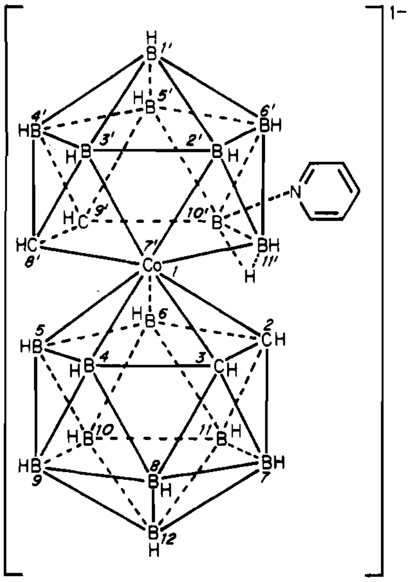
(29) Francis, J. N.; Hawthorne, M. F. *Inorg. Chem.* **1971**, *10* (4), 863–864; *J. Am. Chem. Soc.* **1968**, *90* (6), 1663–1664. St. Clair, D.; Zalkin, A.; Templeton, D. H. *Inorg. Chem.* **1969**, *8* (10), 2080–2086.



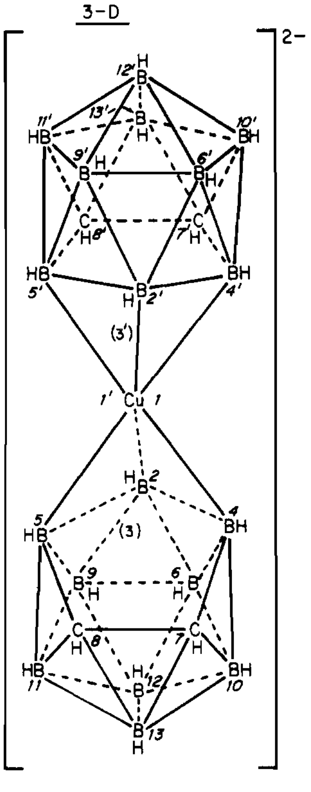
A[25]



B[26]



C[27]



D[28]

A. 2,2′,3,3′-tetracarba-1-nickela[(12v)[I_h-(1551)-Δ^{20}-*closo*]-1-*commo*-1′-(12v)[I_h-(1551)-Δ^{20}-*closo*]tricosaborane](22)

B. 1,1-dichlorodocosahydro[2,2′,3,3′-tetracarba-1-urana[(12v)[I_h-(1551)-Δ^{20}-*closo*]-1-*commo*-1′-(12v)[I_h-(1551)-Δ^{20}-*closo*]tricosaborate]](2−)

C. 10′,11′-μ-hydro-1′,2,2′,3,3′,4,4′,5,5′,6,6′,7,8,8′,9,9′,10,11,11′,12-icosahydro-10′-(pyridine)-[2,3,8′,9′-tetracarba-1-cobalta[(12v)[I_h-(1551)-Δ^{20}-*closo*]-1-*commo*-7′-(11v)[I_h-(1551)-Δ^{20}-*closo*(−1v)^{12}]docosaborate]](1−) (component with the greater number of vertices is cited and numbered first)

D. docosahydro[7,7′,8,8′-tetracarba-1-cupra[(12v)[C_{2v}-(1$v^4$22$v^6$422)-Δ^{22}-*closo*(−1v)^3]-1-*commo*-1′-(12v)[C_{2v}-(1$v^4$22$v^6$422)-Δ^{22}-*closo*(−1v)^3]tricosaborate]](2−)

Figure 3. Monocommo *conjuncto*-polyboron hydrides.

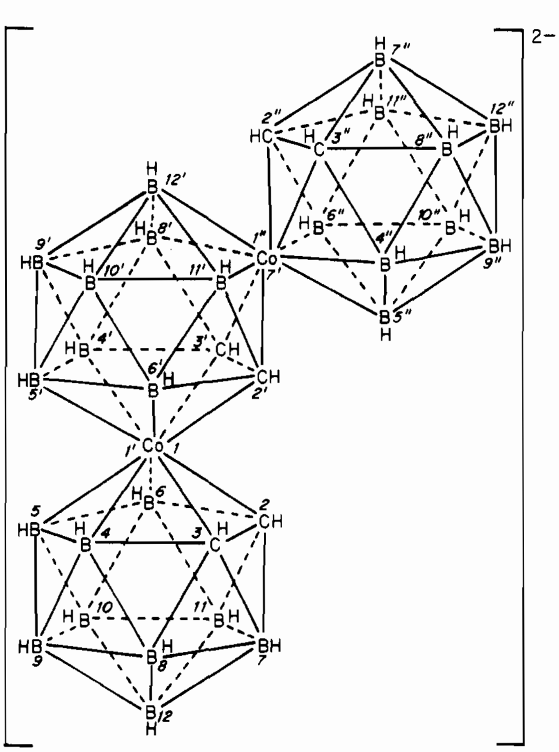
only by one common vertex, are readily described by our recommended method as illustrated by the compound in Figure 4 and by the compound in Figure E of the supplementary material.

"Spiro" Method. In the special situation in which a monocommo compound consists of two identical skeletal structures, the method given in the current rules[5b,6b] based on a technique for naming certain organic spiro ring systems[7c] can be adapted advantageously just as ring assembly techniques can be adapted for certain *conjuncto*-polyboron hydrides connected by boron–boron bonding as discussed above. Although the term "commo" was used in the current rules for *conjuncto*-polyboron hydrides, the format for spiro ring systems consisting of identical components was retained. Accordingly, but with the modifications suggested above, compounds A, B, and D in Figure 3 could be named as follows:[30]

3A: 2,2′,3,3′-tetracarba-1-nickela-1,1′-*commo*-bi[(12v)[I_h-(1551)-Δ^{20}-*closo*]dodecaborane](22)

3B: 1,1-dichlorodocosahydro[2,2′,3,3′-tetracarba-1-urana-1,1′-*commo*-bi[(12v)[I_h-(1551)-Δ^{20}-*closo*]dodecaborate]](2−)

3D: docosahydro[7,7′,8,8′-tetracarba-1-cupra-1,1′-*commo*-bi[(12v)[C_{2v}-(1$v^4$22$v^6$422)-Δ^{22}-*closo*(−1v)^3]dodecaborate]](2−)



dotriacontahydro[2,2′,2″,3,3′,3″-hexacarba-1,7′-dicobalta-[(12*v*)[I_h-(1551)-Δ^{20}-*closo*]-1-*commo*-1′-(12*v*)[I_h-(1551)-Δ^{20}-*closo*]-7′-*commo*-1″-(12*v*)[I_h-(1551)-Δ^{20}-*closo*]-tetratriacontaborate]](2−)

Figure 4. A poly(monocommo) *conjuncto*-polyboron hydride.[29]

It should be noted that the numbering in the names for 3A and 3B above is not the same as it would be according to the current rules because here the common vertex has been given preference for lowest locants, as discussed above.

The unsymmetrical compound C in Figure 3[31] can be derived from a symmetrical monocommo structure. Accordingly, it could be described by using the "debor"[1b] method as follows: 5′,10′-*μ*-hydro-2,2′,3,3′,4,4′,5,5′,6,7,7′,8,8′,9,9′,10,11,11′,-12,12′-icosahydro-10′-(pyridine)[2,2′,3,11′-tetracarba-1-cobalta-6′-debor-1,1′-*commo*-bi[(12*v*)[I_h-(1551)-Δ^{20}-*closo*]-docosaborate]](1−). Note that the numbering of the nonclosed component for this name is not as shown for compound C in Figure 3; being derived from an icosahedron, the common atom is assigned the lowest locant and the debor position the highest possible locant, i.e., (6′).

Extending the method given in the current rules[5b,6b] to poly(monocommo) systems consisting of identical components is possible only by accepting the suggested modifications discussed above. In addition, a numerical prefix could also be added to the commo term to indicate the number of single common vertices. Hence, the compound in Figure 4 could be named dotriacontahydro[2,2′,2″,3,3′,3″-hexacarba-1,7′-dicobalta-1,1′:7′,1″-bis(*commo*)-ter[(12*v*)[I_h-(1551)-Δ^{20}-*closo*]dodecaborate]](2−).

conjuncto-Polyboron Hydrides with Components Sharing Two or More Common Atoms (Structures D and E in Figure 1)

Recommended Linking Descriptor Method. *conjuncto*-Polyboron hydrides consisting of two component polyhedra or polyhedral fragments with two (edge-fused) or three adjacent common vertices are named by using the terms "dicommo" or "tricommo", respectively, in the *link notation* in place of commo as shown by the examples in Figures 5–7 and in Figures F and G of the supplementary material.

The names for the three isomers of the dicommo octadecaborane(22) shown in Figure 5 demonstrate the importance of the basic numbering principles discussed above. In particular, by requiring each polyhedron or polyhedral fragment to be oriented and numbered independently, clockwise or anticlockwise, so that the vertices connecting the components have the lowest locants possible, it is possible to specify and differentiate structural isomers and enantiomers in a manner fully consistent with established principles of stereochemical nomenclature.[7f] Thus, *n*-$B_{18}H_{22}$[32] (shown as A in Figure 5) is differentiated from *iso*-$B_{18}H_{22}$[33] (shown as B in Figure 5) by the locant sequence for the common vertices, i.e., -2,4...4′,2′- vs. -2,4...2′,4′-, respectively. The enantiomers B(1) and B(2) in Figure 5 have the same locant sequence for their common vertices,[34] in agreement with a basic principle of stereochemical nomenclature.[7f] These enantiomers are distinguished by giving the direction of numbering for each component. We have used the capital italic letters *C*, for clockwise, and *A*, for anticlockwise. Thus, stereoisomer B(1) in Figure 5 is the *CC* enantiomer, and B(2) the *AA* enantiomer. To be fully consistent with principles of stereochemical nomenclature, these descriptors should precede the full name. A third stereoisomer of *iso*-$B_{18}H_{22}$, having the "open" side of both polyhedral fragments on the same side, is achiral and can be differentiated from the enantiomeric pair by the directional descriptor *AC*-.

The tetradecaborane(20)[35] shown in Figure 6 is named as a "dicommo" polyborane according to our recommended method as shown by structure A in Figure 6; it can also be named as a nonclosed polyborane derived from a 17-vertex polyhedron[1b] as shown by structure B in Figure 6.

The only known example that could be considered as a *conjuncto*-polyboron hydride with more than three common vertices is $B_{20}H_{16}$[37] whose skeletal structure is described in an earlier paper as one polyhedron.[1c] As a tetracommo system, it could be described by our recommended procedure as follows: 2*H*,3*H*,4*H*,5*H*-[(12*v*)[C_{2v}-($1v^4 22v^6 422$)-Δ^{22}-*closo*-$(-1v)^1$]-2,3,4,5-*tetracommo*-4′,5′,2′,3′-(12*v*)[C_{2v}-($1v^4 22v^6 422$)-Δ^{22}-*closo*$(-1v)^1$]icosaborane](16).

Fusion Method. The current rules of boron nomenclature provide names for the octadecaborane(22) isomers shown in Figure 5[5a,6a] and the tricommo structure shown in Figure 7 by adapting principles used for naming fused-ring systems;[7b] i.e., the components are cited separately, one being considered

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(30) According to the current rules[5b,6b] heteroatom prefixes and hydro ligands are cited with the separate component. The format we suggest here increases the flexibility of the method by eliminating the need for these features to be symmetrically positioned in a compound.

(31) As far as we know, the only attempt to apply the current rules for naming an unsymmetrical monocommo system was made for this structure[27a] as follows: (3,11′)-*commo*-[undecahydro-1,2-dicarba-3-cobalta-*closo*-dodecaborato][decahydro-9′-pyridyl-7′,8′-dicarba-11′-cobalta-*nido*-undecaborate](1−).

(32) Simpson, P. G.; Lipscomb, W. N. *Proc. Natl. Acad. Sci. U.S.A.* **1962**, *48*, 1490–1491. *J. Chem. Phys.* **1963**, *39* (1), 26–34. Pitochelli, A. R.; Hawthorne, M. F. *J. Am. Chem. Soc.* **1962**, *84* (16), 3218.

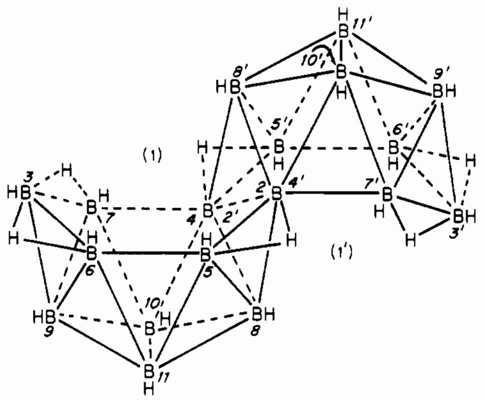
(33) Simpson, P. G.; Folting, K.; Dobrott, R. D.; Lipscomb, W. N. *J. Chem. Phys.* **1963**, *39* (9), 2339–2348.

(34) In the current rules,[5a,6a] these enantiomers have different locant sequences for their common vertices because polyhedral or polyhedral fragment components had to be numbered clockwise.

(35) Huffman, J. C.; Moody, D. C.; Schaeffer, R. *J. Am. Chem. Soc.* **1975**, *97* (6), 1621–1622.

(36) Enemark, J. H.; Friedman, L. B.; Lipscomb, W. N. *Inorg. Chem.* **1966**, *12* (5), 2165–2173.

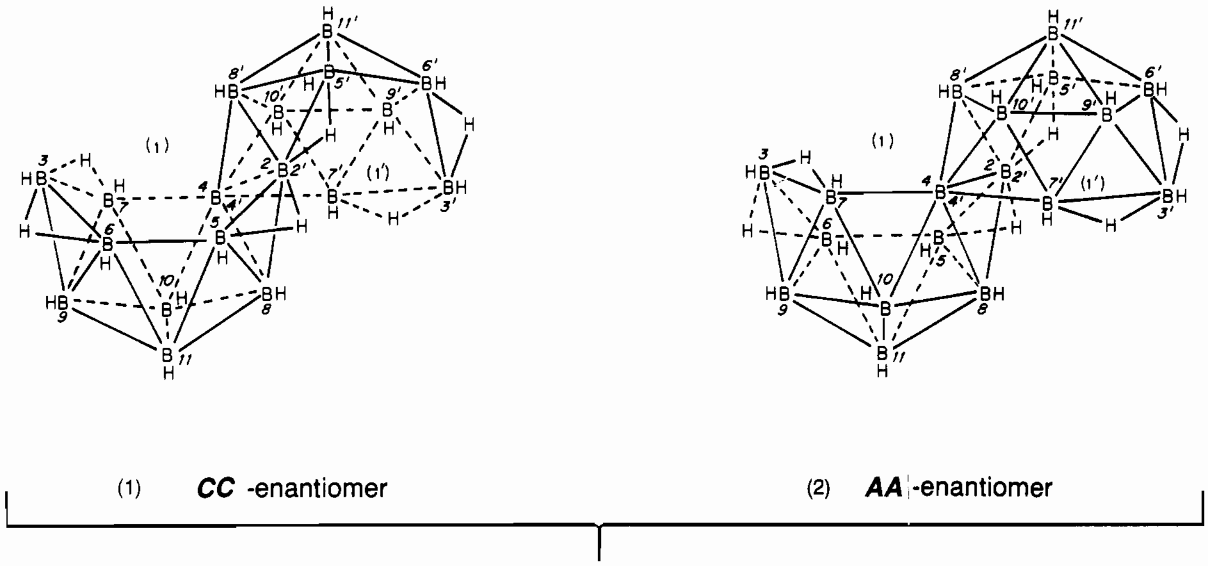
(37) Dobrott, R. D.; Friedman, L. B.; Lipscomb, W. N. *J. Chem. Phys.* **1964**, *40* (3), 866–872. Miller, N. E.; Forstner, J. A.; Muetterties, E. L. *Inorg. Chem.* **1964**, *3* (12), 1690–1694. Miller, N. E.; Muetterties, E. L. *J. Am. Chem. Soc.* **1963**, *85* (21), 3506. Friedman, L. B.; Dobrott, R. D.; Lipscomb, W. N. *J. Am. Chem. Soc.* **1963**, *85* (21), 3505.



A^{32}

A. (2,5-μ*H*),(3,6-μ*H*),(3′,6′-μ*H*),(3,7-μ*H*),(3′,7′-μ*H*),-(4,5′-μ*H*)[(10*v*)[C_{2v}-($1v^{6}2v^{4}422$)-Δ^{18}-*closo*(−1*v*)^{1}]-2,4-*dicommo*-4′,2′-(10*v*)[C_{2v}-($1v^{6}2v^{4}422$)-Δ^{18}-*closo*(−1*v*)^{1}]-octadecaborane](22)

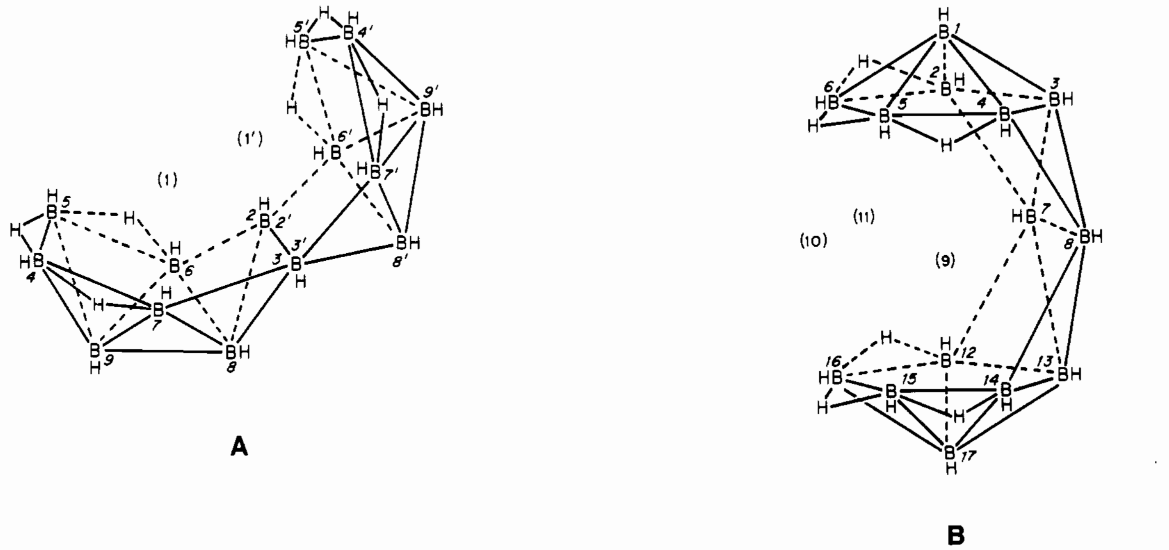
B. (2,5-μ*H*),(2,5′-μ*H*),(3,6-μ*H*),(3′,6′-μ*H*),(3,7-μ*H*),-(3′,7′-μ*H*)[(10*v*)[C_{2v}-($1v^{6}2v^{4}422$)-Δ^{18}-*closo*(−1*v*)^{1}]-2,4-*dicommo*-2′,4′-(10*v*)[C_{2v}-($1v^{6}2v^{4}422$)-Δ^{18}-*closo*(−1*v*)^{1}]-octadecaborane](22)



(1) ***CC*** -enantiomer (2) ***AA*** -enantiomer

B^{33}

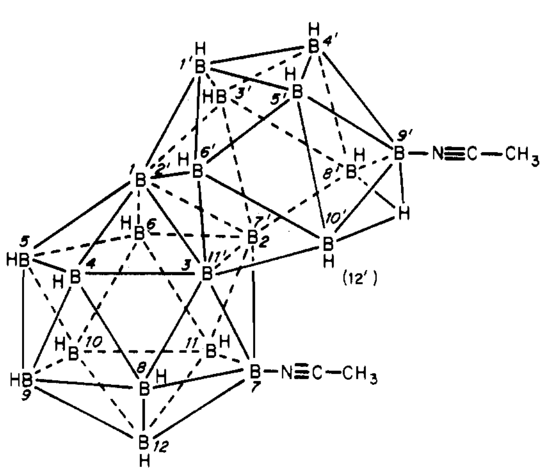
Figure 5. Octadecaborane(22) isomers: dicommo *conjuncto*-polyboranes.



A. 2*H*,3*H*-(4,5-μ*H*),(4′,5′-μ*H*),(4,7-μ*H*),(4′,7′-μ*H*),(5,6-μ*H*),(5′,6′-μ*H*)[(8*v*)[C_{2v}-($1v^{6}4v^{4}22$)-Δ^{14}-*closo*(−1*v*)^{1}]-2,3-*dicommo*-2′,3′-(8*v*)[C_{2v}-($1v^{6}4v^{4}22$)-Δ^{14}-*closo*(−1*v*)^{1}]tetradecaborane](20)

B. (2,6-μ*H*),(4,5-μ*H*),(5,6-μ*H*),(12,16-μ*H*),(14,15-μ*H*),(15,16-μ*H*)[(14*v*)[D_{5h}-($155v^{6}51$)-Δ^{30}-*closo*(−3*v*)^{9,10,11}]tetradecaborane](20)

Figure 6. Tetradecaborane(20):[35] a dicommo *conjuncto*-polyborane.



7,9′-bis(acetonitrile-*N*)(8′,9′,10′-μ_3H)[7,9′-didehydro[(12*v*)[I_h-(1551)-Δ^{20}-*closo*]-1,2,3-*tricommo*-2′,7′,11′-(11*v*)[I_h-(1551)-Δ^{20}-*closo*(−1*v*)^{12}]icosaborane]](16)

Figure 7. A tricommo *conjuncto*-polyboron hydride.[36]

as a base component and the other cited as a prefix. The common atoms of each component are noted by sets of locants separated by a colon and inserted, within brackets, between the components. The disadvantage of this technique, as discussed before,[1a,b] is that the actual number of skeletal atoms and heteroatoms or the number and position of hydrogen atoms in a neutral hydride are not obvious from the name.[11] For organic compounds this is not a real problem, but for polyboron hydrides, where numerical prefixes denote the number of skeletal atoms and heteroatoms and arabic numbers give the number of hydrogen atoms, it can be a disconcerting difficulty. Within these limitations, the published technique can be used both with descriptor names and with nido or arachno names; however, for the latter, these semisystematic descriptors can refer only to the skeletal structure; positions of extra and bridging hydrogen atoms implied for the isolated nonclosed structure[1b] cannot be assumed. Some of the disadvantages noted above can be alleviated by following the same modification to current methods suggested above for assembly names. In addition we would urge the use of the numbering techniques as suggested here. Thus, the following modified "fusion names" are possible for the $B_{18}H_{22}$ isomers in Figure 5:

5A: (5,7′-μH),(6,7-μH),(8,9-μH),(8′,9′-μH),(9,10-μH),(9′,10′-μH)[*nido*-decaborano[6′,5′:5,6]-*nido*-decaborane](22)

5B: (6,7-μH),(6′,7′-μH),(8,9-μH),(8′,9′-μH),(9,10-μH),(9′,10′-μH)[*nido*-decaborano[5′,6′:5,6]-*nido*-decaborane](22)

Note that these names use "nido" numbering,[1b] which is not the numbering shown in Figure 5.

If the positions of the bridging hydrogens in the nido component of the multi(polyhedral) system in Figure 6 are ignored, as recommended above, a semisystematic fusion name can be written as follows: 3*H*,8*H*-(4,5-μH),(4′,5′-μH),(5,6-μH),-(5′,6′-μH),(6,7-μH),(6′,7′-μH)[*nido*-octaborano[3′,8′:3,8]-*nido*-octaborane](20). Note the use of "nido" numbering[1b] in these names, not the numbering shown in Figure 6.

The current rules extend the fusion principles adapted for edge-fused systems to face-fused systems.[5d,6d] Incorporating the modifications discussed above would result in names like the following for the compound in Figure 7: 7,9′-bis(acetonitrile-*N*)(8′,9′,10′-μ_3H)[7,9′-didehydro-*nido*-undecaborano[2′,7′,11′:1,2,3](12*v*)[I_h-(1551)-Δ^{20}-*closo*]dodecaborane](16).

conjuncto-Polyboron Hydrides with Components Connected by Bridging Hydrogen Atoms (Structure F in Figure 1)

Recommended Linking Descriptor Method. Another type of *conjuncto*-polyboron hydride structure readily included within the scope of our proposal is that in which the components are connected by bridging hydrogen atoms. We suggest the designation "μH" be used in the link notation in place of the colon and "commo" term used in the notations for *conjuncto*-polyboron hydride structures discussed above as shown for structure F in Figure 1. Two connecting bridging hydrogens could be indicated by "di-μH" or "μH_2", preceded and followed by pairs of locants just like for the "dicommo" structures described in the preceding section.[38] The compounds in Figure 8 illustrate this type of *conjuncto* system.

In forming the names for these compounds, we have chosen to treat the skeletal atoms connected by bridging hydrogen atom(s) in the same manner as other "connected" vertices in *conjuncto* systems; i.e., we have assumed that there are no other hydrogen atoms on these skeletal atoms. Further, hydrogen atoms bridging between components have been included in the parenthetical arabic number following the name of the polyborane, as shown by compound B in Figure 8, even though they are also cited as part of the descriptor. However, in names of ionic polyboron hydrides, bridging hydrogen atoms have not been cited additionally as hydro ligands, as shown by compound A in Figure 8.

Multiplicative Method. The current rules of boron nomenclature utilize a technique[5e,6e] that is quite similar to the "assembly-type" names discussed above. Although this method is useful when the polyboron hydride is ionic and the components are identical, there does not appear to be a clear-cut way to apply it to a neutral polyboron hydride. Applying the same modifications to current methods suggested above for assembly names would lead to the following name for the ionic compound A in Figure 8: 1,2′-μ-hydro-octadecahydrobis-[(10*v*)[D_{4d}-(1441)-Δ^{16}-*closo*]decaborate](2−).

Finally, there are some important questions regarding *conjuncto* systems connected by bridging atoms or groups other than hydrogen atoms. For example, presumably a bridging hydrogen in a neutral structure could be substituted; however, it would appear that some guidelines would have to be developed for ionic compounds. Hence, for now, we have no specific recommendations for handling the rare *conjuncto* systems where components are connected by bridging atoms or groups other than hydrogen.

Complex *conjuncto*-Polyboron Hydrides

There are a few *conjuncto*-polyboron hydride structures known today that do not fit nicely into one of the three types discussed above. Two of these are shown in Figure 9.

Compound A in Figure 9 may be considered as a "monocommo" system with an additional boron–boron connection. Hence, the name given is a combination of two formats discussed above; note that we have chosen to cite the

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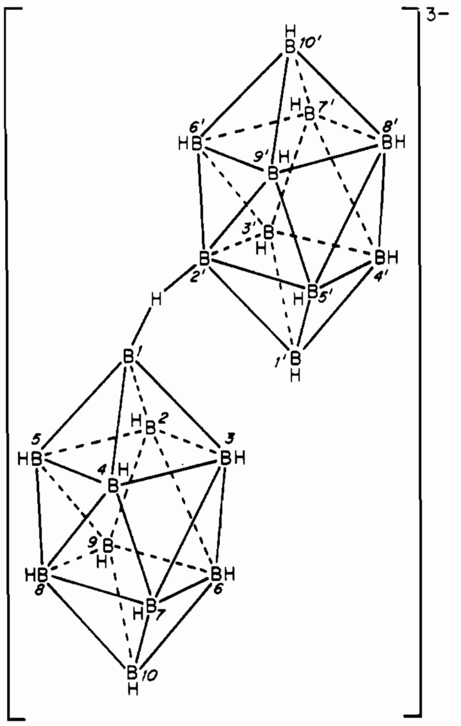
(38) An alternate format would be to cite the bridging hydrogens separately, as for example, (1-μH-3′)(3-μH-1′).

(39) Chamberland, B. L.; Muetterties, E. L. *Inorg. Chem.* **1964**, *3* (10), 1450–1456. Hawthorne, M. F.; Piling, R. L.; Stokely, P. F.; Garrett, P. M. *J. Am. Chem. Soc.* **1963**, *85* (22), 3704–3705. Lipscomb, W. N. *Proc. Natl. Acad. Sci. U.S.A.* **1961**, *47*, 1791–1795.

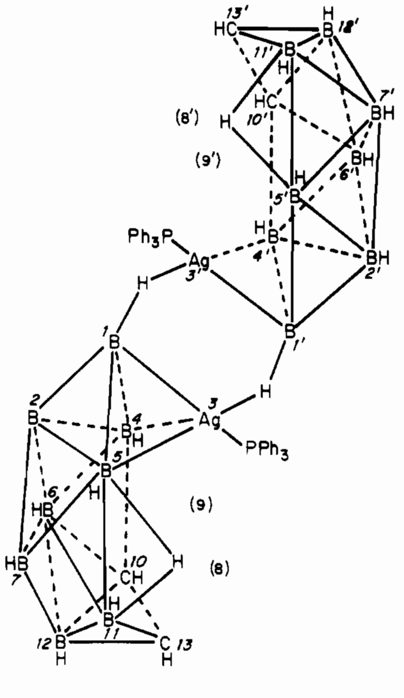
(40) Colquhoun, H. M.; Greenhough, T. J.; Wallbridge, M. G. H. *J. Chem. Soc., Chem. Commun.* **1980**, 192–194.

(41) Finster, D. C.; Sinn, E.; Grimes, R. N. *J. Am. Chem. Soc.* **1981**, *103* (6), 1399–1407.

(42) Maxwell, W. M.; Sinn, E.; Grimes, R. N. *J. Am. Chem. Soc.* **1976**, *98* (12), 3490–3495.



A[39]



B[40]

A. octadecahydro[(10*v*)[D_{4d}-(1441)-Δ^{16}-*closo*]-1-μH-2′-(10*v*)[D_{4d}-(1441)-Δ^{16}-*closo*]icosaborate](3−)

B. 3,3′-bis(triphenylphosphine)(5,11-μH),(5′,11′-μH)[10,10′,13,13′-tetracarba-3,3′-diargenta[(11*v*)[C_{2v}-(1$v^4$22$v^6$422)-Δ^{22}-*closo*(−2*v*)^{8,9}]-1,3-di-μH-3′,1′-(11*v*)[C_{2v}-(1$v^4$22$v^6$422)-Δ^{22}-*closo*(−2*v*)^{8,9}]docosaborane]](20)

Figure 8. *conjuncto*-Polyboron hydrides connected by bridging hydrogen atoms.

"commo" description first in the linking notation.[43]

Compound B in Figure 9 can be named as a "dicommo" system between two capped (7*v*)[D_{5h}-(151)-Δ^{10}-*closo*] polyhedra, as given. Although this name is perhaps the most consistent with our proposals as given in this paper, there are several other ways to describe this structure. First, it can be described as a "monocommo" system between a (7*v*)[D_{5h}-(151)-Δ^{10}-*closo*] polyhedron and its capped homologue plus the prefix "dicyclo". If the polyhedron with four heteroatoms is chosen as the capped polyhedron, the following name can be derived: 2-(η^5-cyclopentadienyl)-4,4′,5,5′-tetramethyl-[4,4′,5,5′-tetracarba-2-cobalta-1-ferra-4′,8:5′,8-dicyclo-[(7*v*)[D_{5h}-(151)-Δ^{10}-*closo*(+1*v*)^{1,2,3}]-1-*commo*-1′-(7*v*)[D_{5h}-(151)-Δ^{10}-*closo*]tetradecaborane]](12). Note that, in this name, the positions indicated by the "cyclo" prefixes are preferred to the heteroatoms for numbering.

Secondly, compound B in Figure 9 can be viewed as a "monocommo" system between two (7*v*)[D_{5h}-(151)-Δ^{10}-*closo*] polyhedra that is capped by a five-coordinate "BH" vertex. This is very analogous to the description of this structure in the literature.[42] Since the "BH" vertex is capping a monocommo structure, it would seem most logical to denote this by adding our capping notation[1a] after the complete "*commo*" descriptor as follows:[44] 2-(η^5-cyclopentadienyl)-4,4′,5,5′-tetramethyl[4,4′,5,5′-tetracarba-2-cobalta-1-ferra[(7*v*)[D_{5h}-(151)-Δ^{10}-*closo*]-1-*commo*-1′-(7*v*)[D_{5h}-(151)-Δ^{10}-*closo*]-(+1*v*)$^{1,2,2',3,3'}$]tetradecaborane](12).

Thirdly, compound B in Figure 9 can be described as a tetradebor derivative of a (17*v*)[D_{5h}-(155$v^6$51)-Δ^{30}-*closo*] polyhedron with an internally bridging iron atom. The problem here is the method for indicating the internally bridging iron atom. To include it as part of the descriptor would produce a name such as 2-(η^5-cyclopentadienyl)-4,5,14,15-tetramethyl[4,5,14,15-tetracarba-2-cobalta-18-ferra[(14*v*)[D_{5h}-(155$v^6$51)-Δ^{30}-*closo*(−4*v*)^{8,9,10,11}(+1*v*)μ_{11}(*i*)]-tetradecaborane]](12).[45] To cite the iron atom as a bridging prefix would give a name such as 2-(η^5-cyclopentadienyl)-4,5,14,15-tetramethyl[4,5,14,15-tetracarba-2-cobalta-μ_{11}-iron[(13*v*)[D_{5h}-(155$v^6$51)-Δ^{30}-*closo*(−4*v*)^{8,9,10,11}]tetradecaborane]](12).

Polyboron Hydride Structures with Bridging Vertices ("Edge Capping")

During the course of our work on the development of a structural nomenclature for polyboron hydrides, several structures have been encountered whose description would be made easier by including a notation in our descriptor for vertices bridging an edge of a polyhedron or a polyhedral fragment. For this purpose we propose to use to same format

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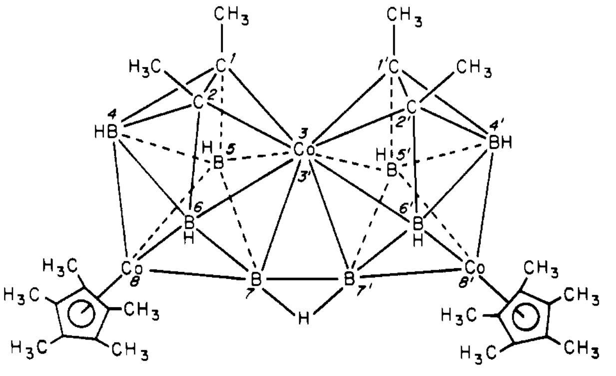
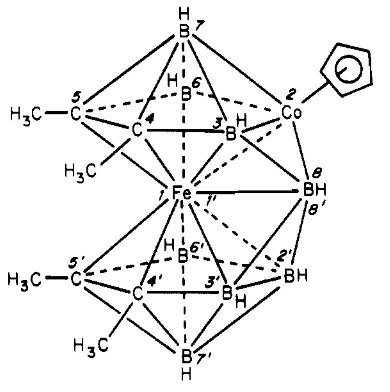
(43) The prefix "cyclo", introduced in an earlier paper as a method for forming an additional edge in a polyhedron or polyhedral fragment,[1b] could also be used to name compound A in Figure 9 as follows: 1,1′,2,2′-tetramethyl-8,8′-bis(pentamethyl-η^5-cyclopentadienyl)-(7,7′-μH)[1,1′,2,2′-tetracarba-3,8,8′-tricobalta-7,7′-cyclo[(8*v*)[D_{2d}-(2222)-Δ^{12}-*closo*]-3-*commo*-3′-(8*v*)[D_{2d}-(2222)-Δ^{12}-*closo*]hexadecaborane]]-(11). As before,[1b] the use of cyclo does not affect the assumptions regarding the presence or absence of hydrogen atoms on the skeletal atoms at each end of the new connection.

(44) In a previous paper[1a] we had also suggested the alternative method of describing a capping vertex as a prefix. The resulting name, compound B in Figure 9, would be 2-(η^5-cyclopentadienyl)-4,4′,5,5′-tetramethyl-[4,4′,5,5′-tetracarba-2-cobalta-1-ferra-1,2,2′,3,3′-bor[(7*v*)[D_{5h}-(151)-Δ^{10}-*closo*]-1-*commo*-1′-(7*v*)[D_{5h}-(151)-Δ^{10}-*closo*]tetradecaborane]](12).

(45) Other formats are entirely possible, for example, (+1*v*μ_{11}), (+1*v*)$^{\mu_{11}}$, (+1*v*)$^{\mu(i)}$, [+1(μ_{11})*v*], and we encourage comments and other suggestions.



A[41]

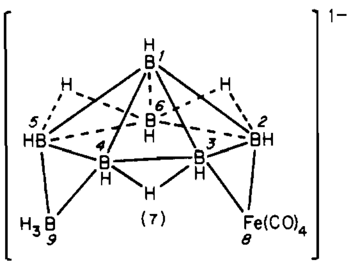


B[42]

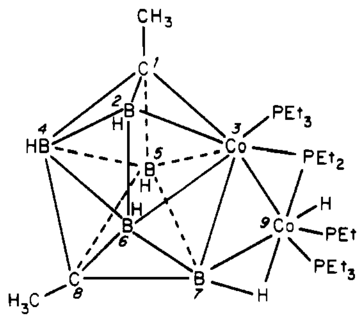
A. 1,1′,2,2′-tetramethyl-8,8′-bis(pentamethyl-η^5-cyclopentadienyl)-(7,7′-*μH*)[1,1′,2,2′-tetracarba-3,8,8′-tricobalta[(8*v*)[D_{2d}-(2222)-Δ^{12}-*closo*]-(3-*commo*-3′)(7:7′)-(8*v*)[D_{2d}-(2222)-Δ^{12}-*closo*]hexadecaborane]](11)

B. 2-(η^5-cyclopentadienyl)-4,4′,5,5′-tetramethyl-8*H*-[4,4′,5,5′-tetracarba-2-cobalta-1-ferra[(8*v*)[D_{5h}-(151)-Δ^{10}-*closo*$(+1v)^{1,2,3}$]-1,8-*dicommo*-1′,8′-(8*v*)[D_{5h}-(151)-Δ^{10}-*closo*$(+1v)^{1,2,3}$]tetradecaborane]](12)

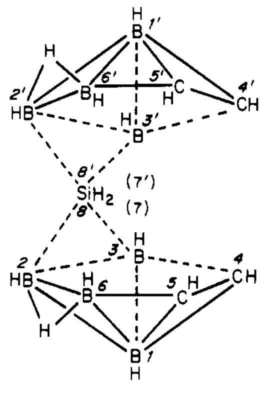
Figure 9. Complex *conjuncto*-polyboron hydrides.



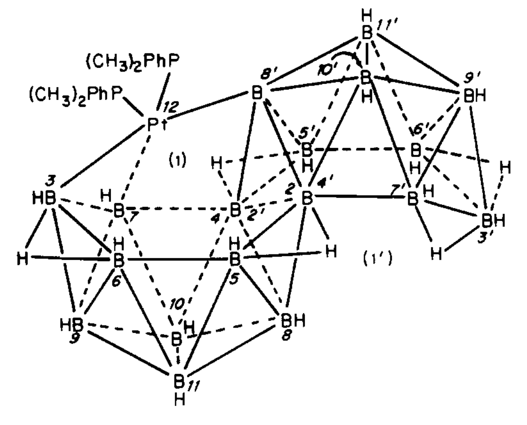
A[46]



B[47]



C[48]



D[49]

A. 8,8,8,8-tetracarbonyl-2,6:3,4:5,6-tri-*μ*-hydro-1,2,3,4,5,6,9,9,9-nonahydro[8-ferra[(8*v*)[D_{5h}-(151)-Δ^{10}-*closo*$(-1v)^7(+2v)^{2,3:4,5}$]octaborate]](1−)

B. 3,9-*μ*-(diethylphosphino)-9-hydrido-1,8-dimethyl-3,9,9-tris(triethylphosphine)(7,9-*μH*)[7-dehydro-1,8-dicarba-3,9-dicobalta[(9*v*)[D_{2d}-(2222)-Δ^{12}-*closo*$(+1v)^{3,7}$]nonaborane]](6)

C. 8*H*,8*H*-(2,6-*μH*),(2′,6′-*μH*)[4,4′,5,5′-tetracarba-8-sila[(7*v*)[D_{5h}-(151)-Δ^{10}-*closo*$(-1v)^7(+1v)^{2,3}$]-8-*commo*-8′-(7*v*)[D_{5h}-(151)-Δ^{10}-*closo*$(-1v)^7(+1v)^{2,3}$]tridecaborane]](16)

D. 12,12-bis(dimethylphenylphosphine)(2,5-*μH*),(3,6-*μH*),(3′,6′-*μH*),-(3′,7′-*μH*),(4,5′-*μH*)[8′-dehydro-12-platina[[(10*v*)[C_{2v}-($1v^6 2v^4$422)-Δ^{18}-*closo*$(-1v)^1$]-2,4-*dicommo*-4′,2′-(10*v*)[C_{2v}-($1v^6 2v^4$422)-Δ^{18}-*closo*$(-1v)^1$]$(+1v)^{3,7,8'}$]nonadecaborane]](20)

Figure 10. "Edge-capped" polyboron hydrides.

as described in our earlier paper for capping vertices.[1a] A vertex bridging an edge of a polyhedron or polyhedral fragment is described by a symbol that consists of an arabic number equal to the number of bridging vertices added, preceded by the plus sign (indicating addition) and followed by the italic letter *v* (for "vertex"), all enclosed in parentheses, added to the descriptor for the polyhedron or polyhedral fragment after the term "*closo*" or the symbolism for vertex removal. The positions of the bridging vertices are given by appropriate pairs of locants for the edges that are bridged. These locants are cited as superscripts outside the parentheses and are separated by a colon. Examples of polyboron hydride structures illustrating "edge capping" are shown in Figure 10.

Compound A in Figure 10 illustrates this procedure for a nonclosed polyboron hydride described in an earlier paper by means of bridging prefixes or a debor descriptor.[1b] Compound B in Figure 10 shows a recently reported compound in which

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(46) Mangion, M.; Clayton, W. R.; Hollander, O.; Shore, S. G. *Inorg. Chem.* **1977**, *16* (8), 2110–2114.

a vertex bridges an edge of a closed polyhedral structure. It shows the value of including the bridging cobalt atom as an integral part of the heteropolyboron structure. If this cobalt atom were described as a ligand bridge, the bridging ligands between the dodecahedron and the cobalt atom could not be specifically described under present rules.

Compound C in Figure 10 illustrates a *conjuncto*-polyboron hydride analogue that could be named as a "monocommo" system between two edge-capped polyhedral fragments as shown. To us, this name is easier to visualize than one based on a $(7\upsilon)[D_{3h}\text{-}(33\upsilon^{4}3)\text{-}\Delta^{14}\text{-}\mathit{closo}(-2\upsilon)^{8,9}]$ polyhedral fragment.

The recently reported compound shown as D in Figure 10 demonstrates that the capping technique we proposed could be extended to partial capping. Without such an extension, this structure would have to be treated as a cyclo–edge capped–dicommo system or a seco–tricommo system, both of which result in much more complex names.

Coordination Nomenclature for *conjuncto*-Metallopolyboron Hydrides

As for closed and nonclosed metallopolyboron hydrides,[1b] principles of coordination nomenclature may be applied for naming certain *conjuncto*-polyboron hydrides by using the methods developed in this and earlier papers[1] to specify the structure of the polyboron hydride fragments as ligands. Coordination names for such compounds in this paper (D in Figure 2; A, B, C, and D in Figure 3; Figure 4; A and D in Figure 10) and compounds II in Figure A and II in Figure D of the supplementary material are listed in Table A in the supplementary material; ligand numberings, where needed, are shown in Figure H in the supplementary material.

Summary

Nomenclature for *conjuncto*-polyboron hydrides, i.e., polyboron hydride structures consisting of two or more polyhedra or polyhedral fragments and their hetero analogues and derivatives, has been proposed on the basis of the descriptor system developed earlier for closed, capped closed, and nonclosed polyboron hydrides. Limitations of methods given in current rules are discussed. The descriptor method for capped closed polyhedra developed earlier is extended to include bridging vertices (edge capping) and internal bridging atoms.

Supplementary Material Available: Table A, giving coordination names for some *conjuncto*-polyboron hydrides, Figures A–G, showing additional structures and names of *conjuncto*-polyboron hydrides, and Figure H, giving ligand numberings for the coordination names in Table A (12 pages). Ordering information is given on any current masthead page.

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(47) Barker, G. K.; Garcia, M. P.; Green, M.; Stone, F. G. A.; Parge, H. E.; Welch, A. J. *J. Chem. Soc., Chem. Commun.* **1982**, 688–689.

(48) Tabereaux, A.; Grimes, R. N. *J. Am. Chem. Soc.* **1972**, *94* (13), 4768–4770.

(49) Cheek, Y. M.; Greenwood, N. N.; Kennedy, J. D.; McDonald, W. S. *J. Chem. Soc., Chem. Commun.* **1982**, 80–81.

Contribution from the Materials and Molecular Research Division, Lawrence Berkeley Laboratory, and Department of Chemistry, University of California, Berkeley, California 94720

Preparation of Tertiary Phosphine Complexes of Tetravalent and Trivalent Uranium Methyltrihydroborates. Crystal Structures of Tetrakis(methyltrihydroborato)(1,2-bis(dimethylphosphino)ethane)uranium(IV) and Tris(methyltrihydroborato)bis(1,2-bis(dimethylphosphino)ethane)uranium(III)

JOHN BRENNAN, RON SHINOMOTO, ALLAN ZALKIN,* and NORMAN EDELSTEIN*

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$(CH_3BH_3)_4U[(CH_3)_2PCH_2CH_2P(CH_3)_2]$ and $(CH_3BH_3)_3U[(CH_3)_2PCH_2CH_2P(CH_3)_2]_2$ have been synthesized and their molecular structures determined by single-crystal X-ray diffraction. The space groups, unit cell parameters, and R factors are as follows: $(CH_3BH_3)_4U[(CH_3)_2PCH_2CH_2P(CH_3)_2]$, monoclinic, $P2_1/c$, a = 9.439 (3) Å, b = 14.023 (4) Å, c = 16.596 (2) Å, β = 97.48 (4)°, Z = 4, d_x = 1.536 g/cm^3, R = 0.024 ($F^2 > 3\sigma(F^2)$); $(CH_3BH_3)_3U[(CH_3)_2PCH_2CH_2P(CH_3)_2]_2$, tetragonal, $P4_32_12$, a = 11.297 (4) Å, c = 23.03 (2) Å, Z = 4, d_x = 1.412 g/cm^3, R = 0.024 ($F^2 > 3\sigma(F^2)$). Both complexes are unimolecular in the crystalline state. The uranium(IV) atom is coordinated to four BH_3CH_3 groups through tridentate hydrogen bridges and to two P atoms of the $(CH_3)_2PCH_2CH_2P(CH_3)_2$ ligand. The uranium(III) complex is coordinated to three BH_3CH_3 groups through tridentate hydrogen bridges and to four P atoms from the $(CH_3)_2PCH_2CH_2P(CH_3)_2$ ligands. The U–B distances for the U(IV) and U(III) complexes average 2.57 ± 0.01 and 2.63 ± 0.02 Å, respectively; the U–P distances for the U(IV) and U(III) complexes average 3.02 ± 0.01 and 3.13 ± 0.06 Å, respectively.

Introduction

Four Lewis base etherate adducts of $U(BH_4)_4$ have been structurally characterized and shown to display a variety of structural types.[1] $U(BH_4)_4$ also forms adducts with other Lewis bases, but these compounds have not been isolated.[2] A number of U(III) tetrahydroborate complexes have recently been reported. Marquet-Ellis et al. have thermally decomposed $U(BH_4)_4$ in toluene solution and reacted the $U(BH_4)_3$ formed by this process with crown ethers to form soluble compounds.[3] Wasserman et al. have isolated and structurally characterized $U(BH_4)_3(DMPE)_2$ (DMPE = 1,2-bis(dimethylphosphino)ethane) and $U(BH_4)_3(Ph_2Ppy)_2$ (Ph_2Ppy = 2-(diphenylphosphino)pyridine) from the reactions of $U(BH_4)_3(THF)_x$ (THF = tetrahydrofuran) with the appropriate ligands.[4] An

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(1) (a) Rietz, R. R.; Zalkin, A.; Templeton, D. H.; Edelstein, N. M.; Templeton, L. K. *Inorg. Chem.* **1978**, *17*, 653. (b) Rietz, R. R.; Edelstein, N. M.; Ruben, H. W.; Templeton, D. H.; Zalkin, A. *Inorg. Chem.* **1978**, *17*, 658. (c) Zalkin, A.; Rietz, R. R.; Templeton, D. H.; Edelstein, N. M. *Inorg. Chem.* **1978**, *17*, 661.

(2) Rietz, R. R., unpublished results.

(3) Dejean-Meyer, A.; Folcher, G.; Marquet-Ellis, H. *J. Chim. Phys. Phys.-Chim. Biol.* **1983**, *80*, 579.

(4) (a) Wasserman, H. J.; Moody, D. C.; Ryan, R. R. *J. Chem. Soc., Chem. Commun.* **1984**, 532. (b) Wasserman, H. J.; Moody, D. C.; Paine, R. T.; Ryan, R. R.; Salazar, K. V. *J. Chem. Soc., Chem. Commun.* **1984**, 533.