Contribution from Chemical Abstracts Service, Columbus, Ohio 43210,
and the Department of Chemistry, The University of Chicago, Chicago, Illinois 60637

Structural Nomenclature for Polyboron Hydrides and Related Compounds. 2. Nonclosed Structures

JAMES B. CASEY,[1a] WILLIAM J. EVANS,[1b] and WARREN H. POWELL*[1a]

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Methods based on principles developed previously for closed polyboron hydrides are proposed for uniquely describing nonclosed polyboron hydrides. The principles of the descriptor system for uniquely describing capped closed polyboron polyhedra previously reported are applied to polyhedral fragments.

Introduction

In the preceding paper,[2a] we showed how a method for definitively describing the structures of closed polyboron polyhedra[2b–c] can be used conveniently to provide a structural nomenclature for fully triangulated polyboron hydrides and their hetero analogues and derivatives. In this report we consider structural nomenclature for nonclosed, or open, polyboron hydrides, whose structures can be visualized as fragments of closed polyboron hydride polyhedra. Two approaches are presented: (1) semisystematic, using the descriptive terms *nido* and *arachno*, and (2) systematic, based on *derivation* of the nonclosed polyboron hydride structure from a closed polyboron structure. Two methods are suggested for the systematic approach: (a) use of the prefix "debor"[3a] with the name of the closed polyboron hydride derived as described in the preceding paper[2a] and (b) derivation of the polyhedral fragment within the descriptor itself in a manner quite analogous to the method suggested for describing capped polyboron polyhedra in the preceding paper.[2a]

A variety of terms have been used to describe nonclosed polyboron hydrides. The descriptor *nido-* was introduced to denote "almost closed" polyhedral structures to contrast with the descriptor *closo-*.[3b,4a] The imprecise nature of this definition led, inevitably, to its use for all nonclosed polyboron hydrides,[5] despite efforts to introduce other prefixes to differentiate among various types of nonclosed polyboron hydride structures, for example, *arachno-*,[6] *hypho-*,[7,8a] *canasto-*,[9] and *anello-*.[9] Hence, the descriptor *nido-* probably can never have an unambiguous specific structural meaning but only a general one of nonclosed.

Attempts have been made to give the descriptors *nido-* and *arachno-* precise definitions. First, they were related stoichiometrically to nonclosed polyboranes of the general formulas B_nH_{n+4} and B_nH_{n+6},[6a,b] respectively, and then to polyboron hydrides with $2n + 4$ and $2n + 6$ "skeletal electrons",[10] respectively. Such relationships have been discussed extensively in the literature.[11] Although these definitions were apparently quite adequate early in the development of polyboron hydride chemistry, an increasing number of instances are occurring where these relationships are ambiguous and therefore these descriptors are no longer generally applicable.[12] For example, two B_9H_{15} isomers are known,[15,16] both of which are arachno by either definition. And, octaborane(12),[17] which is nido according to both of the above definitions, is considered by many to be structurally arachno (see below). Further, a number of exceptions to structures predicted on the basis of skeletal electron count have now been observed,[18] most notably in heteropolyboron hydrides. In addition, *different* geometries have been reported for some heteropolyboron hydride compounds that have the same skeletal electron count.[19a] Thus, it seems quite certain that factors other than skeletal electron count may significantly affect the geometry of a polyboron hydride, especially in heteropolyboron hydride systems.[18–20]

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(1) (a) Chemical Abstracts Service. (b) The University of Chicago; Camille and Henry Dreyfus Teacher-Scholar. Present address: Department of Chemistry, University of California, Irvine, CA 92717.

(2) (a) Casey, J. B.; Evans, W. J.; Powell, W. H. *Inorg. Chem.*, preceding paper in this issue. (b) *Ibid.* **1981**, *20* (5), 1334–1341. (c) *Ibid.* **1981**, *20* (10), 3556–3561.

(3) International Union of Pure and Applied Chemistry. "Nomenclature of Inorganic Boron Compounds", *Pure Appl. Chem.* **1972**, *30* (3–4), 638–170: (a) Rule 3.221, pp 687–688; (b) Rule 2.4, p 686; (c) Rule 5.1, p 693.

(4) American Chemical Society. "The Nomenclature of Boron Compounds", *Inorg. Chem.* **1968**, *7* (10), 1945–1964: (a) Rule 1.6, p 1947; (b) Rules 2.321–2.322, p 1948; (c) Rule 7.1, p 1952.

(5) For example, see: Williams, R. E. *Prog. Boron Chem.* **1969**, *2*, 51–52, 59, 62. Muetterties, E. L. *Pure Appl. Chem.* **1972**, *29* (4), 585–595. Štibr, B.; Baše, K.; Plešek, J.; Heřmånek, S.; Dolanský, J.; Janoušek, Z. *Ibid.* **1977**, *49*, 803–811, Note a, p 803. Bowser, J. R.; Grimes, R. N. *J. Am. Chem. Soc.* **1978**, *100* (14), 4623–4624, footnote 12.

(6) (a) Williams, R. E. *U.S. NTIS, AD Rep.* **1969**, *AD-689380*, 3–4 (Technical Report 17). (b) Williams, R. E. In "The 1970 McGraw-Hill Yearbook of Science and Technology"; McGraw-Hill: New York, 1970, pp 132–134. (c) Williams, R. E. *Inorg. Chem.* **1971**, *10* (1), 210–214.

(7) Rudolph, R. W.; Thompson, D. A. *Inorg. Chem.* **1974**, *13* (12), 2779–2782, footnote 22.

(8) (a) Williams, R. E. *Adv. Inorg. Chem. Radiochem.* **1976**, *18*, 81; (b) *Ibid.* **1976**, *18*, 67–142.

(9) Stumpf, W. In "Themen zur Chemie des Bors"; Möllinger, H., Ed.; Dr. Alfred Hüthig Verlag GmbH: Heidelberg, 1976; pp 85–119; *Chem. Z.* **1975**, *99* (1), 1–12. "Gmelin Handbuch der anorganischen Chemie", 8 Aufl.; Springer-Verlag: Berlin, 1974; Ergänzungswerk, Band 15, Borverbindungen 2 (Kapitel 1, S. 1–138), p 25.

(10) (a) Wade, K. *Chem. Commun.* **1971**, 792–793; "Electron Deficient Compounds"; Nelson: London, 1971; *Inorg. Nucl. Chem. Lett.* **1972**, *8*, 559, 563, 823; *Nature (London), Phys. Sci.* **1972**, *240*, 71; *New Sci.* **1974**, *62*, 615. (b) Rudolph, R. W.; Pretzer, W. R. *Inorg. Chem.* **1972**, *11* (8), 1974–1978. (c) Mingos, D. M. . *Nature* (*London*), *Phys. Sci.* **1972**, *236*, 99–102.

(11) For example, see: Wade, K. *Adv. Inorg. Chem. Radiochem.* **1976**, *18*, 4–7, 10–16. Reference 8b, above.

(12) Even the descriptor *closo-* has not been considered fully adequate to describe closed, i.e., fully triangulated, heteropolyboron systems. The term "hypercloso" has been introduced[13] to distinguish closed systems with $2n$ skeletal electrons from those with $2n + 2$ skeletal electrons and "isocloso" has been used[14] to differentiate a C_{3v}-hexadecahedron from the common D_{4d}-hexadecahedron.

(13) Jung, C. W.; Baker, R. T.; Knobler, C. B.; Hawthorne, M. F. *J. Am. Chem. Soc.* **1980**, *102* (18), 5782–5790. Jung, C. W.; Baker, R. T.; Hawthorne, M. F. *Ibid.* **1981**, *103* (4), 810–816.

(14) Bould, J.; Greenwood, N. N.; Kennedy, J. D.; McDonald, W. S. *J. Chem. Soc., Chem. Commun.* **1982**, 465–467.

(15) Dickerson, R. E.; Wheatley, P. J.; Howell, P. A.; Lipscomb, W. N. *J. Chem. Phys.* **1957**, *27* (1), 200–209. Kotlensky, W. V.; Schaeffer, R. *J. Am. Chem. Soc.* **1958**, *80* (17), 4517–4519. Simpson, P. G.; Lipscomb, W. N. *J. Chem. Phys.* **1964**, *35* (4), 1340–1343. Burg, A. B.; Kratzer, R. *Inorg. Chem.* **1962**, *1* (4), 725–730.

(16) (a) Dobson, J.; Keller, P. C.; Schaeffer, R. *J. Am. Chem. Soc.* **1965**, *87* (15), 3522–3523; *Inorg. Chem.* **1968**, *7* (3), 399–402. (b) Keller, P. C. *Ibid.* **1970**, *9* (1), 75–78. (c) Moody, D. C.; Schaeffer, R. *Ibid.* **1976**, *15* (1), 233–236.

(17) Enrione, R. E.; Boer, F. P.; Lipscomb, W. N. *Inorg. Chem.* **1964**, *3* (12), 1659–1666. Rietz, R. R.; Schaeffer, R.; Sneddon, L. G. *Ibid.* **1972**, *11* (6), 1242–1244.

(18) (a) Grimes, R. N.; Sinn, E.; Pipal, J. R. *Inorg. Chem.* **1980**, *19* (7), 2087–2095. (b) O'Neill, M. E.; Wade, K. *Ibid.* **1982**, *21* (1), 461–464.

(19) (a) Zimmerman, G. J.; Sneddon, L. G. *Inorg. Chem.* **1980**, *19* (12), 3650–3655. (b) Zimmerman, G. J.; Hall, L. W.; Sneddon, L. G. *Ibid.* **1980**, *19* (12), 3642–3650.

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Although these descriptive terms may provide a way of classifying structures generically, they cannot be considered adequate to describe specific structures, at least according to stoichiometric or electronic definitions.[21]

Another approach to defining descriptive terms for polyhedral fragments more precisely was to relate their definitions to the known homologous series of idealized closed polyhedral polyboron hydrides by removal of vertices.[6c,9,10b] In general, the terms *nido*- and *arachno*- were defined to describe polyhedral fragments with one "open", i.e., nontriangular, face derived by the removal of one and two vertices, respectively, from the known homologous series of idealized, closed polyhedral polyboron hydrides.[22] As such, however, except for the rather simple and highly symmetrical polyhedra, these descriptive terms carry little, if any, specific structural information. To achieve more structural specificity, the definitions of *nido*- and *arachno*- were refined by specifying the removal of particular vertices. Thus, *nido*- was restricted to polyhedral fragments formed by the removal of one "highest coordination vertex" from a particular closed polyboron hydride[23] and *arachno*- was restricted to polyhedral fragments formed by removal of a "highest coordination vertex" from the open face of a nido structure.[6c,10b] These refined definitions accounted for the skeletal structures of the nonclosed polyboron hydrides known at the time, except for the isomeric nonaborane(15)[16] generated by the removal of a low coordination vertex from the open face of the $B_{10}H_{14}$ structure.[25] However, two arachno structures can be generated from the polyhedral structures of $[B_9H_9]^{2-}$ and $[B_{10}H_{10}]^{2-}$ by removing a "highest coordination vertex" from the open face of a nido structure. Hence, the definition of *arachno*- was further refined[26] by adding the requirement that an *arachno*- polyhedral fragment must have a minimum number of vertices of "order 2", where the "order" of a vertex is the number of nearest-neighbor vertices within the framework of the polyhedron. However, this refinement still did not resolve the problem of the two nonaborane(15) isomers.[15,16] Furthermore, as noted above for nido, the meaning of arachno is being generalized despite the attempts to structurally define its use. For example, the term *arachno* has been used recently to describe polyhedral fragments generated by the removal of two nonadjacent vertices from closed polyhedra.[27,28] Other descriptors such as *canasto* and *anello* have also been used for certain polyhedral fragments.[29,31]

None of the definitions for the descriptors discussed above have proved general enough to form the basis of a comprehensive system for unambiguous description of nonclosed polyboron hydride structures. There are a number of reasons for this. First, although the use of isoarachno[25] provides for distinguishing between the two known isomers of nonaborane(15),[15,16] isomeric structures can be derived from closed polyhedra that cannot be so differentiated. For example, only two of the three isomeric open structures generated by removal of two adjacent vertices from the closed $[B_9H_9]^{2-}$ or $[B_{10}H_{10}]^{2-}$ polyhedra can be described by the descriptors *arachno*- and *isoarachno*-. Similarly, *nido*- and *isonido*- can describe the two open structures derived from the $[C_{2v}\text{-}(1v^{6}2v^{4}422)\text{-}\Delta^{18}\text{-}\mathit{closo}]$ polyhedron by removal of the "highest" and "lowest" coordination vertex, respectively; but removal of a five-coordination vertex cannot be described. This problem will only become more serious with larger and less symmetrical polyhedra. Second, there is octaborane(12),[17] which is nido according to the stoichiometric and electronic definitions but can only be described as nido structurally by derivation from the $[C_{2v}\text{-}(1v^{6}4v^{4}22)\text{-}\Delta^{14}\text{-}\mathit{closo}]$nonaboron polyhedron which is not one of the series of closed polyhedra prescribed for derivation of nonclosed polyboron hydride structures.[6c,10b]

The skeletally isostructural compounds $B_{10}H_{14}$ and $[B_{10}H_{14}]^{2-}$ illustrate a third problem in the use of *nido*- and *arachno*- descriptors. Decaborane(14)[32] is nido by stoichiometric and electronic definitions and is structurally nido by derivation from the closed $[C_{2v}\text{-}(1v^{6}2v^{4}422)\text{-}\Delta^{18}\text{-}\mathit{closo}]$-undecaboron polyhedron; however, it is arachno in structure relative to the icosahedron. Tetradecahydrodecaborate(2−) is arachno by the electronic definition and can be derived structurally from the icosahedral dodecaboron polyhedron, but it is also structurally nido with respect to the $[C_{2v}\text{-}(1v^{6}2v^{4}422)\text{-}\Delta^{18}\text{-}\mathit{closo}]$undecaboron polyhedron noted above. Hence, for these 10-vertex nonclosed structures, different electron counts result in the same structure, and therefore the same skeletal structure can be considered as both nido and arachno.

Some of these difficulties can be circumvented by continuing to allow only one polyhedron for each B_n polyboron hydride to be used as the reference polyhedron for precisely defining descriptive terms; however, other nonclosed structures derived from these polyhedra would still have to be described. Other problems could be resolved by precisely defining the structure of the closed polyhedral system to which a descriptive term applies, for example, by the method proposed in our earlier reports,[2b,c] and designating specific vertices to which the operations prescribed by the descriptor are applied. However, this method would result in names just like those derived by the "debor" method, which is described below, except that the prefixes *nido*-, *arachno*-, etc. would be used instead of the debor prefix. Since the debor names are straightforward without residual implications of structural, stoichiometric, or electronic meaning, they should clearly be preferred.

Since there does not seem to be a general method for describing structures of nonclosed polyboron hydrides and related compounds using descriptive terms as prefixes, we propose the following ways for naming such polyboron compounds. These suggestions should not interfere with the use of descriptive terms such as *nido*- and *arachno*- for describing classes of different nonclosed polyboron hydrides in a general (generic)

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(20) Cox, D. N.; Mingos, D. M. P. *J. Chem. Soc., Dalton Trans.* **1981**, 1788–1797. Brint, P.; Healy, E. F.; Spalding, T. R.; Whelan, T. *Ibid.* **1981**, 2515–2522.

(21) The descriptor *hypho*- was introduced[7,8a] to describe B_nH_{n+8} polyboranes, or polyboranes with $2n + 8$ "skeletal electrons". While only a few polyboron hydrides of this class have been reported, it seems quite certain that the same problems in specifying structure will appear as discussed in this report for *nido*- and *arachno*-.

(22) It is interesting to note here that the concept of such a structural relationship for "nido" seems to have been recognized in the first published official rules of boron nomenclature by an alternate procedure for numbering nonclosed ("open") boron frameworks lacking only one vertex from being a closed polyboron hydride.[4b]

(23) The descriptor *isonido*- was introduced recently[24] to describe a 10-vertex polyhedral fragment formally derived from the $[C_{2v}\text{-}(1v^{6}2v^{4}422)\text{-}\Delta^{18}\text{-}\mathit{closo}]$ polyhedron by removal of a four ("lowest") coordination vertex.

(24) Crook, J. E.; Greenwood, N. N.; Kennedy, J. D.; McDonald, W. S. *J. Chem. Soc., Chem. Commun.* **1981**, 933–934.

(25) The descriptor *isoarachno*- was recently introduced[24] to describe a carbanonaborane(14) with this particular structure.

(26) Rudolph, R. W. *Acc. Chem. Res.* **1976**, *9*, 446–452.

(27) Finster, D. C.; Grimes, R. N. *J. Am. Chem. Soc.* **1981**, *103* (10), 2675–2683.

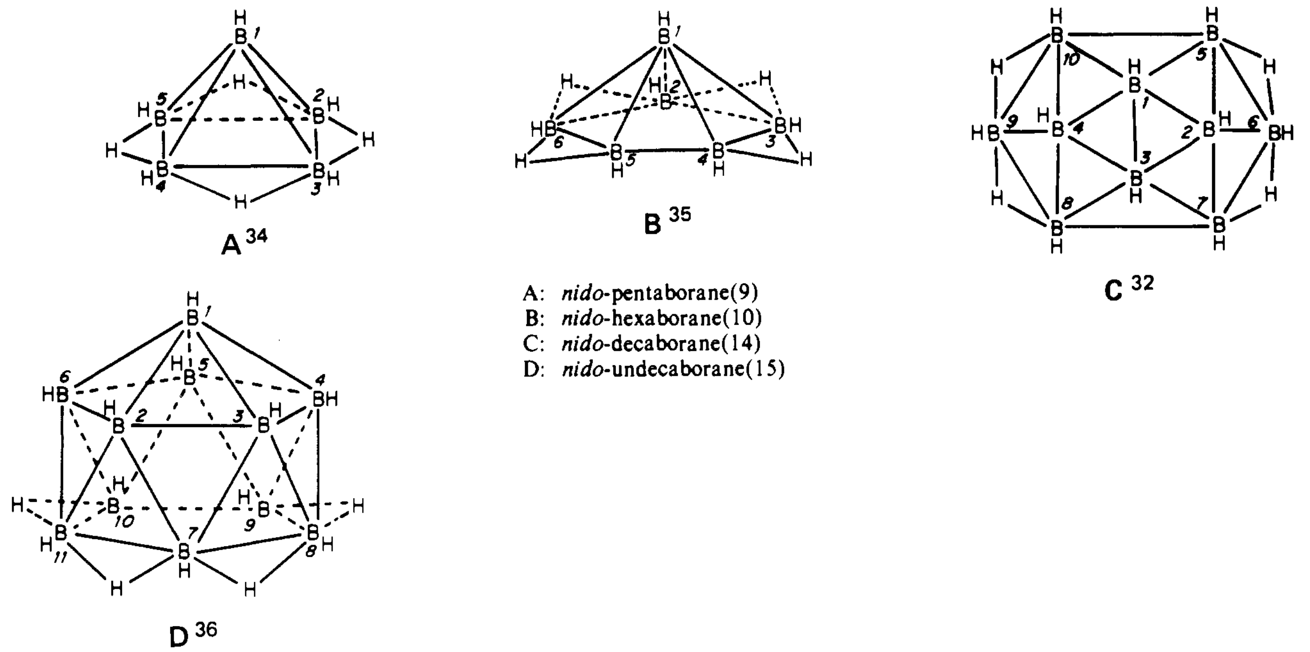
(28) Siwapinyoyos, G.; Onak, T. *Inorg. Chem.* **1982**, *21* (1), 156–163.

(29) The descriptor *canasto*-, apparently derived from the name canastide[30] used to derive a trivial name for the anion $[C_2B_8H_{10}]^{4-}$, has been defined only generally to describe nonclosed carbaboranes with two "open" (nontriangular) faces having the general shape of a basket with a handle.[9]

(30) Francis, J. N.; Hawthorne, M. F. *Inorg. Chem.* **1971**, *10* (4), 863–864.

(31) The descriptor *anello*- was introduced to describe a ring-shaped structure whose skeletal atoms are arranged in one or two parallel planes such that the addition of two vertices, one on each side of the "ring", would generate a closed structure.[9]

(32) (a) Casper, J. S.; Lucht, C. M.; Harker, D. *Acta Crystallogr.* **1950**, *3*, 436–455. (b) Moore, E. B., Jr.; Dickerson, R. E.; Lipscomb, W. N. *J. Chem. Phys.* **1957**, *27* (1), 209–211. (c) Tippe, A.; Hamilton, W. C. *Inorg. Chem.* **1969**, *8* (3) 464–470.


A[34]

B[35]

C[32]

D[36]

A: *nido*-pentaborane(9)
B: *nido*-hexaborane(10)
C: *nido*-decaborane(14)
D: *nido*-undecaborane(15)

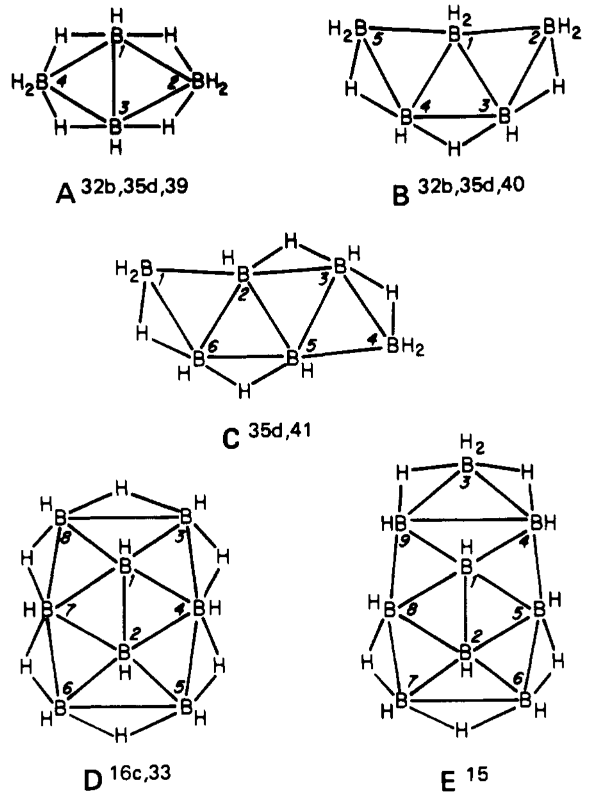
Figure 1. *nido*-Polyboranes (B_nH_{n+4}).

way, very much like the terms alkane and alkene describe particular classes of hydrocarbons.

Semisystematic Names for Nonclosed Polyboron Hydrides

Neutral Polyboron Hydrides. Even though the "debor" technique described below could be used in all cases as shown in Table I of the supplementary material, it seems desirable to retain names and numberings that have become generally accepted in the literature. Therefore, we suggest that the prefixes *nido*- and *arachno*- be used to describe known polyboranes, subject to the following requirements. First, each term must describe only one nonclosed polyborane structure for each B_n composition, where n = 4–11 (inclusive). As a result, each term will be structurally meaningful by definition; for example, *arachno*-B_8H_{14} will refer only to one specific structure.[16c,33] Second, the structure described by *nido* or *arachno* must agree with all of the definitions discussed above, stoichiometric, electronic, and structural (derived from the closed homologous polyboron hydride polyhedra prescribed for use with these descriptors[6c,10b]). Finally, these descriptive prefixes must refer to different skeletal structures when used with the same B_n polyborane. The names, numbering of skeletal atoms, and positions of BH_2 groups and bridging hydrogen atoms for the nine known polyboranes that meet the above conditions are given in Figures 1 and 2. The numbering shown is consistent with that developed for nonclosed polyboranes in the rules for naming boron compounds[3a,4b] and therefore our proposal *involves no change in numbering from current practice*. Hence, *nido*-$B_{10}H_{14}$ describes the structure, the numbering, and the position of the hydrogen atoms as shown in Figure 1C. If the numbering and positions of the hydrogen atoms in these polyboranes is accepted as specified in Figures 1 and 2, *there will no longer be a need for a set of rules to number nonclosed polyboron hydride structures*.

The known polyboranes B_4H_{10},[32b,35d,39] B_5H_9,[34] B_5H_{11},[32b,35d,40] B_6H_{10},[35] and B_6H_{12}[35d,41] are readily incorporated into this proposal as shown in Figures 1 and 2. No nonclosed hepta-


A[32b,35d,39]

B[32b,35d,40]

C[35d,41]

D[16c,33]

E[15]

A: *arachno*-tetraborane(10)
B: *arachno*-pentaborane(11)
C: *arachno*-hexaborane(12)
D: *arachno*-octaborane(14)
E: *arachno*-nonaborane(15)

Figure 2. *arachno*-Polyboranes (B_nH_{n+6}).

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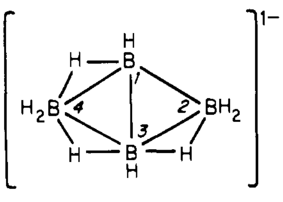
[33] Dobson, J.; Schaeffer, R. *Inorg. Chem.* **1968**, *7* (3), 402–408.

[34] Hedberg, K.; Jones, M. E.; Schomaker, V. *Proc. Natl. Acad. Sci. U.S.A.* **1952**, *38*, 679–686. Dulmage, W. J.; Lipscomb, W. N. *Acta Crystallogr.* **1952**, *5*, 260–264.

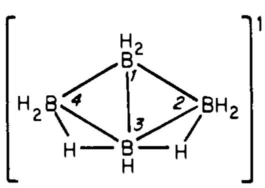
[35] (a) Eriks, K.; Lipscomb, W. N.; Schaeffer, R. *J. Chem. Phys.* **1954**, *22*, 754–755. (b) Hirshfeld, F. L.; Eriks, K.; Dickerson, R. E.; Lippert, E. L., Jr.; Lipscomb, W. N. *Ibid.* **1958**, *28* (1), 56–61. (c) Boone, J. L.; Burg, A. B. *J. Am. Chem. Soc.* **1959**, *81* (7), 1766–1767. (d) Leach, J. B.; Onak, T.; Spielman, J.; Rietz, R. R.; Schaeffer, R.; Sneddon, L. G. *Inorg. Chem.* **1970**, *9* (9), 2170–2175.

[36] A hypothetical parent polyborane, but the basis for naming the $[B_{11}H_{13}]^{2-}$ ion[37] and the important "dicarbollide" ion,[38] $[B_9C_2H_{11}]^{2-}$, and related compounds.

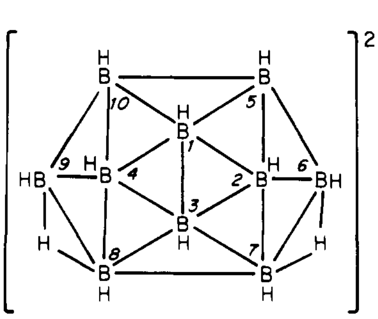
[37] Fritchie, C. F., Jr. *Inorg. Chem.* **1967**, *6* (6), 1199–1203.



A



B



C

A: nonahydro-*arachno*-tetraborate(1−)
B: 2,3:3,4-di-μ-hydro-1,1,2,2,3,4,4-heptahydro-*arachno*-tetraborate(1−)[43]
C: dodecahydro-*nido*-decaborate(2−)

Figure 3. *nido*- and *arachno*-polyboron hydride anions.

boranes, or related compounds, have yet been reported and thus are not included at this time.[42] Should a need arise for semisystematic *nido* and/or *arachno* names for heptaboranes, they could be added provided that the criteria for the use of these names as described above are followed. Octaborane(12)[17] and octaborane(14)[16c,33] have the same skeletal structure, which is arachno according to the accepted structural definition. Since octaborane(14) is also arachno by the stoichiometric and electronic definitions, it is included in this part of our proposal. Octaborane(12) should be named by the systematic "debor" method discussed below. There are two structurally different nonaborane(15) isomers[15,16] that are both arachno according to the stoichiometric and electronic definitions. Only the isomer that is also arachno by the structural definition[15] is included. A *nido*-nonaborane structure is derivable from the [C_{3v}-($1v^{6}3v^{4}33$)-Δ^{16}-*closo*]decaboron polyhedron, but a polyborane with this structure having the proper stoichiometry and skeletal electron count has not yet been reported. Decaborane(14)[32] and undecaborane(15)[36] are nido stoichiometrically and electronically as well as structurally by derivation from the [C_{2v}-($1v^{6}2v^{4}422$)-Δ^{18}-*closo*]undecaboron hydride and icosahedral polyboron hydride skeletons, respectively.

Polyboranes having the same stoichiometry and skeletal structure as those in Figures 1 and 2, but where the position of BH_2 groups and/or bridging hydrogen atoms are different, may also be named as *nido*- or *arachno*-polyboranes, but to be structurally definitive, the positions of all BH_2 groups and bridging hydrogen atoms must be specified by one of the methods described in the preceding paper.[2a] Both methods are illustrated in the debor names for the polyboranes in Figure 4 and in Table I of the supplementary material.

Anionic polyboron hydrides, derived from the neutral *nido*- or *arachno*-polyboranes shown in Figures 1 and 2 by formal removal of hydrogen cations (protons) can be named in a way quite similar to the parent polyboranes. The number of boron atoms is indicated by a numerical prefix added to the anionic name borate (x−), where x is an Arabic number giving the amount of charge. The appropriate descriptive prefix *nido*- or *arachno*- is attached and the hydrogen atoms are designated as ligands in the usual manner; the ligand name hydro is preferred to hydrido.[3c,4c] It is not necessary to add locants for the hydro prefixes unless it is desired to specify the positions of hydrogen atoms in a structure. Some examples are given in Figure 3.

The "Debor" Method for Naming Nonclosed Polyboron Hydrides[3a]

Nonclosed polyboron hydrides may be considered as derived from a closed polyhedral polyboron hydride by the removal of one or more "B" vertices and all of the associated polyhedral edges. The "B" vertices removed are denoted by the subtractive prefix "debor", which, together with the locant of the vertex in the corresponding closed structure, is prefixed to the name of the closed polyhedral boron hydride. The structure of the closed system may be specified by the descriptor as described in our earlier papers.[2b,c] The locants of the skeletal boron atoms of the nonclosed structure are those of the closed polyhedral system from which the nonclosed skeleton was derived. When there is a choice, the highest possible locant is assigned to the debor position. This convention was chosen[3a] in order to keep the numbering of as many nonclosed polyboron hydride structures the same in the "debor" system as previously established by rules for numbering "open" structures.[3a,4b] In this report, when the numbering of the proposed semisystematic *nido*- or *arachno*- structure is not the same as the numbering in the debor system, we have shown the former structure as a projection in the same way as in the boron nomenclature rules;[3,4] when the numbering is the same, the structure is shown only as a three-dimensional polyhedral fragment.

If the nonclosed structure is neutral, the total number of hydrogens of the nonclosed polyborane is indicated by a parenthetical Arabic number added to the end of the name; the position of BH_2 groups and bridging hydrogen atoms are specified by one of the methods described in the preceding paper.[2a] When both BH_2 groups and bridging hydrogen atoms must be specified, in either method the BH_2 groups are indicated first, in ascending order of their locants, followed by the bridging hydrogen atoms. If the nonclosed polyboron hydride is ionic, all hydrogen atoms, including bridging hydrogen atoms, are expressed as hydro[3c,4c] ligands with ap-

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(38) Hawthorne, M. F.; Young, D. C.; Wegner, P. A. *J. Am. Chem. Soc.* **1965**, *87* (8), 1818–1819. Hawthorne, M. F.; Pilling, R. L. *Ibid.* **1965**, *87* (17), 3987–3988. Hawthorne, M. F.; Andrews, T. D. *Chem. Commun.* **1965**, 443–444; *J. Am. Chem. Soc.* **1965**, *87* (11), 2496. Wegner, P. A.; Hawthorne, M. F. *Chem. Commun.* **1966**, 861–862. Warren, L. F., Jr.; Hawthorne, M. F. *J. Am. Chem. Soc.* **1967**, *89* (2), 470–471. Hawthorne, M. F.; Young, D. C.; Andrews, T. D.; Howe, D. V.; Pilling, R. L.; Pitts, A. D.; Reintjes, M.; Warren, L. F., Jr.; Wegner, P. A. *Ibid.* **1968**, *90* (4), 879–896.

(39) Nordman, C. E.; Lipscomb, W. N. *J. Am. Chem. Soc.* **1953**, *75* (16), 4116–4117; *J. Chem. Phys.* **1953**, *21* (10), 1856–1864. Jones, M. E.; Hedberg, K.; Schomaker, V. *J. Am. Chem. Soc.* **1953**, *75* (16), 4116.

(40) Lavine, L. R.; Lipscomb, W. N. *J. Chem. Phys.* **1954**, *22* (4), 614–620.

(41) Gaines, D. F.; Schaeffer, R. *Inorg. Chem.* **1964**, *3* (3), 438–440.

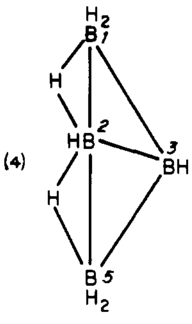
(42) A "nido" structure formally derived from the [D_{2d}-(2222)-Δ^{12}-*closo*]-polyhedron has been used, however, to explain the formation of (trimethylamine)hexahydro-2,4-dicarba-*closo*-heptaboron(1+) ions from *B*-chloro derivatives of 2,4-dicarba-*closo*-heptaborane(7).[28]

(43) Preference for low numbers between bridging and nonbridging hydro ligands has not yet been established in coordination nomenclature rules. Preference in this report has been given arbitrarily to nonbridging ligands. If preference were given to bridging hydro ligands, the semisystematic arachno name would be 1,2:1,4-di-μ-hydro-1,2,2,3,3,4,4-heptahydro-*arachno*-tetraborate(1−).

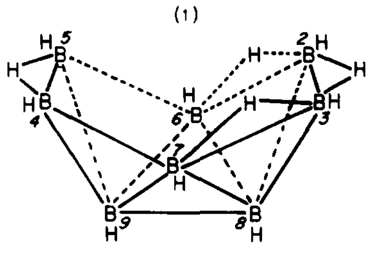
(44) Structure for B_4H_8 in adduct with $(CH_3)_2NPF_2$ according to: La Prade, M. D.; Nordman, C. E. *Inorg. Chem.* **1969**, *8* (8), 1669–1673. See also: Dewar, M. J. S.; McKee, M. L. *Ibid.* **1978**, *17* (6), 1569–1581.

(45) Both methods for indicating "extra" and bridging hydrogen of polyboranes previously described[2a] are given: (i) as prefix symbolism and (ii) as suffix symbolism.

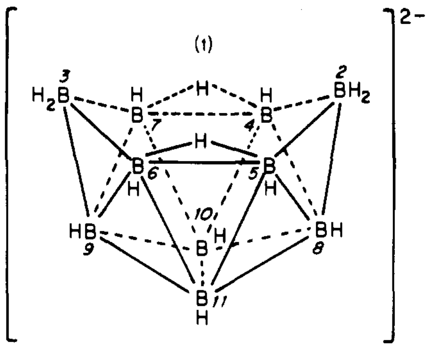
(46) Johnson, H. D., II; Brice, V. T.; Brubaker, G. L.; Shore, S. G. *J. Am. Chem. Soc.* **1972**, *94* (19), 6711–6714.



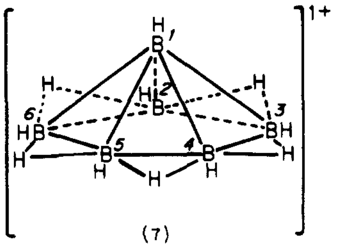
A[44]



B[17]



C



D[46]

A[45] (i): 1*H*,5*H*-(1,2-μH),(2,5-μH)-4-debor[D_{3h}-(131)-Δ^{6}-*closo*]pentaborane(8)
(ii): 4-debor-[D_{3h}-(131)-Δ^{6}-*closo*]pentaborane(8)-1,5-H_2-1,2:2,5-μH_2
B[45] (i): (2,3-μH),(2,6-μH),(3,7-μH),(4,5-μH)-1-debor[C_{2v}-(1$v^6$4$v^4$22)-Δ^{14}-*closo*]-nonaborane(12)
(ii): 1-debor[C_{2v}-(1$v^6$4$v^4$22)-Δ^{14}-*closo*]nonaborane(12)-2,3:2,6:3,7:4,5-μH_4
C (1): tetradecahydro-1-debor[C_{2v}-(1$v^6$2$v^4$422)-Δ^{18}-*closo*]undecaborate(2−)
(2): 4,7:5,6-di-μ-hydro-2,2,3,3,4,5,6,7,8,9,10,11-dodecahydro-1-debor[C_{2v}-(1$v^6$2$v^4$422)-Δ^{18}-*closo*]undecaborate(2−)
D (1): undecahydro-7-debor[D_{5h}-(151)-Δ^{10}-*closo*]heptaboron(1+)
(2): 2,3:2,6:3,4:4,5:5,6-penta-μ-hydro-hexahydro-7-debor[D_{5h}-(151)-Δ^{10}-*closo*]-heptaboron(1+)

Figure 4. "Debor" names for nonclosed polyboron hydrides.

propriate locants, if it is desired to specify the positions of hydrogen atoms in a structure. Debor names for the *nido-* and *arachno-*polyboron hydrides in Figures 1–3 are listed in Table I of the supplementary material; debor names for some other polyboron hydrides are given in Figure 4.

Clearly, debor names for nonclosed polyboron hydrides can be derived from more than one closed structure. Although it really does not matter which closed structure is used as long as it is described and numbered unambiguously, it would seem natural to prefer the closed structure from which the fewest number of vertices would have to be removed. However, it might be more useful on occasion to use a more common closed polyboron hydride structure, even though more polyhedral vertices would have to be removed. For example, the polyborane shown as structure B in Figure 4 might be named as a didebor derivative of the more familiar bicapped square antiprism, as follows: (i) (1,2-μH),(1,4-μH),(2,6-μH),(8,10-μH)-5,9-didebor[D_{4d}-(1441)-Δ^{16}-*closo*]decaborane(12) or (ii) 5,9-didebor[D_{4d}-(1441)-Δ^{16}-*closo*]decaborane(12)-1,2:1,4:2,6:8,10-μH_4.

Nonclosed Heteropolyboron Hydrides

Replacement nomenclature[47a] has been adapted for both neutral and ionic nonclosed heteropolyboron hydrides, including the metallopolyboron hydrides, as it has been adapted for closed heteropolyboron hydrides.[2a] Only if the heteropolyboron hydride has the same skeletal structure and is isoelectronic with a *nido-* or *arachno-*polyboron hydride, should replacement nomenclature be applied to *nido* and *arachno* names (see Figures 1 and 2); therefore, replacement nomenclature with *nido-* or *arachno-*polyboron hydride names for metallopolyboron hydrides should be used with caution. Since the number of hydrogen atoms and the location of bridging hydrogen atoms of a heteropolyborane are generally different from those of the corresponding polyborane, the location of all BH_2 and CH_2 groups, all bridging hydrogen atoms, and any hydrogen on heteroatoms other than carbon in a heteropolyborane must be specified, if known, by one of the methods described in the preceding paper.[2a]

Numbering of nonclosed heteropolyboron hydride structures closely follows the principles given in the preceding paper[2a] for closed heteropolyboron hydride polyhedra. For heteropolyboron hydrides named on the basis of *nido-* or *arachno-*

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(47) 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 B-4, pp 68–70, and Subsection C-0.6, pp 123–127; (b) Rule A-2.6(c), footnote, pp 10–11; Rule C-13.11(e), footnote, p 99, and p 107; (c) Subsection C-0.4, pp 115–117; (d) Rule C-43, pp 116–117.

(48) Baše, K.; Plešek, J.; Heřmánek, S.; Huffman, J.; Ragatz, P.; Schaeffer, R. *J. Chem. Soc., Chem. Commun.* **1975**, 934–935.

(49) Pretzer, W. R.; Rudolph, R. W. *J. Am. Chem. Soc.* **1976**, *98* (6), 1441–1447.

(50) Štíbr, B.; Plešek, J.; Heřmánek, S. *Collect. Czech. Chem. Commun.* **1973**, *38*, 338–342.

(51) A superscript number to the η symbol, e.g., η^5, is used for ligands even when all atoms in a chain or ring are associated with the coordination center. This is consistent with the practice used in CAS index names[52] and much of the current literature; however, the IUPAC Inorganic Nomenclature Rules do not use it.[53a]

(52) "The Naming and Indexing of Chemical Substances for Chemical Abstracts", Appendix IV in "Chemical Abstracts 1977 Index Guide", § 215, pp 1801–1841.

(53) International Union of Pure and Applied Chemistry. "Nomenclature of Inorganic Chemistry (1970)", 2nd ed.; Butterworths: London, 1971: (a) Rule 7.421, pp 49–50; (b) Chapter 7, pp 39–83.

(54) Burg, A. B.; Heinen, H. *Inorg. Chem.* **1968**, *7* (5), 1021–1025.

(55) According to ref 19b, this structure is isoelectronic and isostructural with decaborane(14), and, if so, could be named on the basis of *nido-*decaborane(14) (see Figure 1C) as follows:[45] (i) 2,7-bis(η^5-cyclopentadienyl)-5,6-dimethyl-(8,9-μH),(9,10-μH)-5,6-dicarba-2,7-dicobalta-*nido*-decaborane(10); (ii) 2,7-bis(η^5-cyclopentadienyl)-5,6-dimethyl-5,6-dicarba-2,7-dicobalta-*nido*-decaborane(10)-8,9:9,10-μH_2.

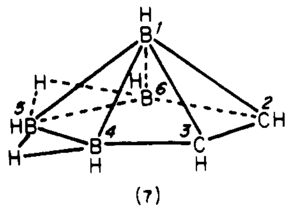
(56) Colquhoun, H. M.; Greenhough, T. J.; Wallbridge, M. G. H. *J. Chem. Soc., Chem. Commun.* **1980**, 192–194.

(57) The determination of the lowest set of locants is a well-established procedure in organic nomenclature.[47b] However, for these nonclosed metallopolyboranes it is necessary to choose the highest locant set for the debor positions. We have done this by reversing the procedure for finding the lowest locant set; i.e., the locant sets were written in *descending* numerical order and compared term by term; the higher locant at the first point of difference determined the higher locant set.

(58) Barker, G. K.; Green, M.; Stone, F. G. A.; Welch, A. J.; Wosley, W. C. *J. Chem. Soc., Chem. Commun.* **1980**, 627–629.

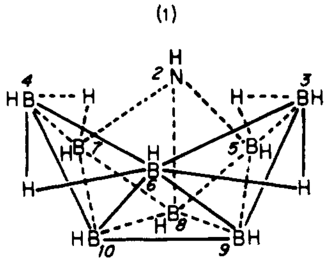
(59) Siedle, A. R.; Todd, L. J. *Inorg. Chem.* **1976**, *15* (11), 2838–2842.

(60) Maxwell, W. M.; Grimes, R. N. *Inorg. Chem.* **1979**, *18* (8), 2174–2178.

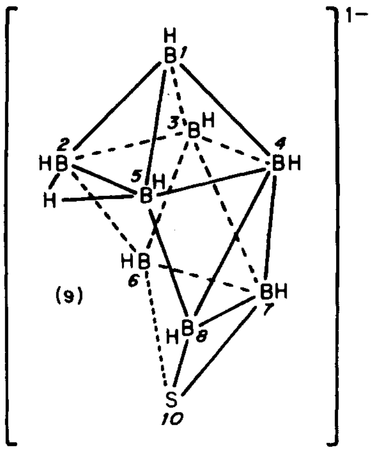


"nido" and "debor" numbering

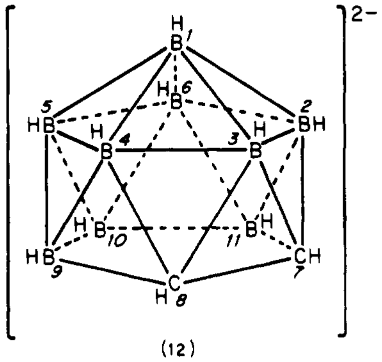
A



B48



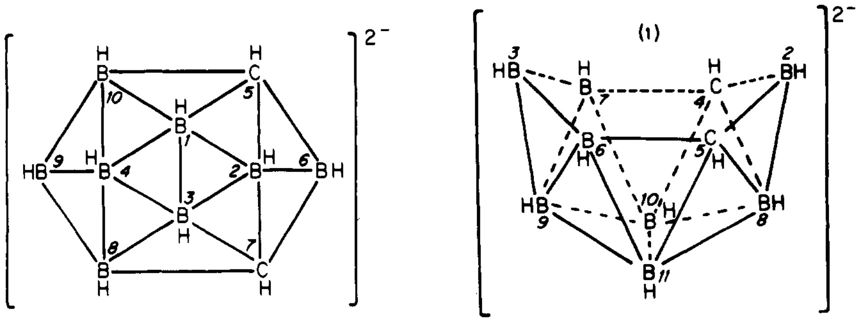
C49



(12)

"nido" and "debor" numbering

D38



(1) "nido" numbering

(2) "debor" numbering

E50

A (1): (4,5-μ*H*),(5,6-μ*H*)-2,3-dicarba-*nido*-hexaborane(8)
(2): (4,5-μ*H*),(5,6-μ*H*)-2,3-dicarba-7-debor[D_{5h}-(151)-Δ^{10}-*closo*]heptaborane(8)
B: 2*H*-(3,5-μ*H*),(3,6-μ*H*),(4,6-μ*H*),(4,7-μ*H*)-2-aza-1-debor[C_{3v}-($1v^{6}3v^{4}33$)-Δ^{16}-*closo*]decaborane(13)
C: 2,5-μ-hydro-octahydro-10-thia-9-debor[D_{4d}-(1441)-Δ^{16}-*closo*]decaborate(1−)
D (1): undecahydro-7,8-dicarba-*nido*-undecaborate(2−)
(2): undecahydro-7,8-dicarba-12-debor[I_h-(1551)-Δ^{20}-*closo*]dodecaborate(2−)
E (1): decahydro-5,7-dicarba-*nido*-decaborate(2−)
(2): decahydro-4,5-dicarba-1-debor[C_{2v}-($1v^{6}2v^{4}422$)-Δ^{18}-*closo*]undecaborate(2−)

Figure 5. Nonclosed heteropolyboron hydrides.

polyboron hydrides, lowest locants are assigned to the heteroatoms consistent with the skeletal structure only; positions of BH_2 groups or bridging hydrogen atoms in the parent polyboron hydride are ignored in assigning numbering priorities. For heteropolyboron hydrides named by the "debor" method, the "debor" position, which must be given the highest possible locant,[3a] is numbered before locants are assigned to skeletal positions of the heteroatoms. When there is still a choice, lowest locants are assigned in the same way as they are for closed heteropolyboron hydrides;[2a] i.e., the locant "1" is assigned to the senior heteroatom, i.e. the heteroatom whose replacement prefix occurs earliest in the list of prefixes given in Table I of the preceding paper.[2a] If more than one heteroatom can have the locant "1", lowest locants are assigned first to the set of heteroatoms, regardless of the kind of heteroatom, and then to the heteroatoms in order of their seniority as given by Table I in the preceding paper.[2a] Examples of nonclosed heteropolyboron hydrides are shown in Figure 5. Both nido (1) and debor (2) names are given, where appropriate.

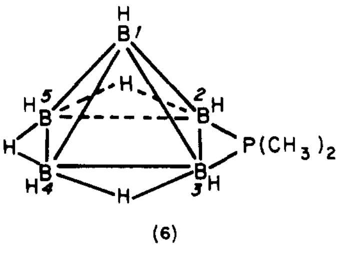
Derivatives of Nonclosed Polyboron and Heteropolyboron Hydrides

Derivatives of nonclosed heteropolyboron hydrides are described in the same way as for closed heteropolyboron compounds in the preceding paper.[2a] Examples of a variety of nonclosed heteropolyboron hydride compounds are given in Figures 6 and 7; both nido (1) and debor (2) names are given, where appropriate. Additional examples may be found in the supplementary material (Figures A and B).

Some nonclosed polyboron and heteropolyboron hydrides are described more conveniently by expressing boron atoms or groups or heteroatoms or heterogroups as substituents or ligands of smaller nonclosed polyboron or heteropolyboron structures, rather than as complete nonclosed structures themselves. For example, the structure shown as A in Figure 6 could be named as a derivative of pentaborane(9) by substituting a bridging hydrogen atom with a phosphino group, as shown. Alternatively, this structure could be named as a nonclosed phosphahexaborane as follows: 7,7-dimethyl-7*H*,7*H*-(2,3-μ*H*),(2,4-μ*H*),(4,5-μ*H*)-7-phospha-6,8-didebor[D_{2d}-(2222)-Δ^{12}-*closo*]octaborane(10). Other examples are given as supplementary material (Figure C).

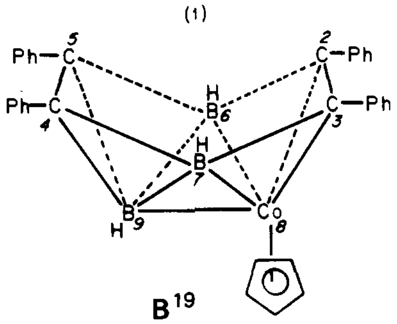
A Descriptor System for Nonclosed Polyboron Hydrides

The "debor" method discussed above for naming nonclosed polyboron hydrides is a subtractive approach requiring that a parent, closed polyhedral polyboron hydride structure be named from which one or more vertices, i.e., boron atoms, are removed by the subtractive prefix "debor". One disadvantage

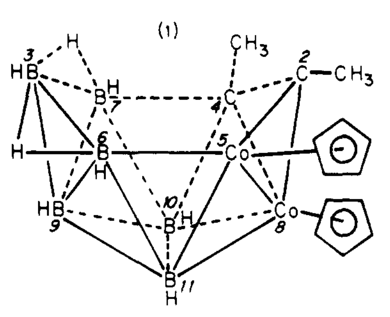


"nido" and "debor" numbering

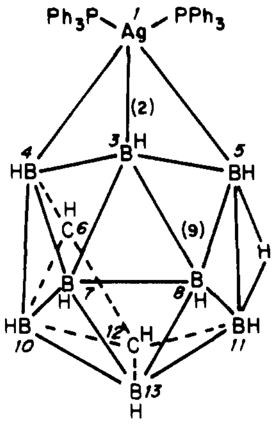
A[54]



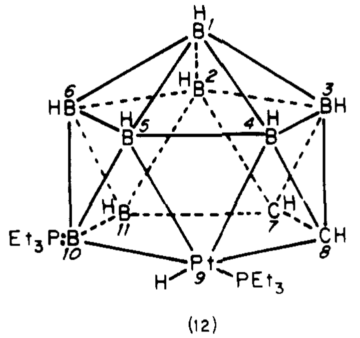
B[19]



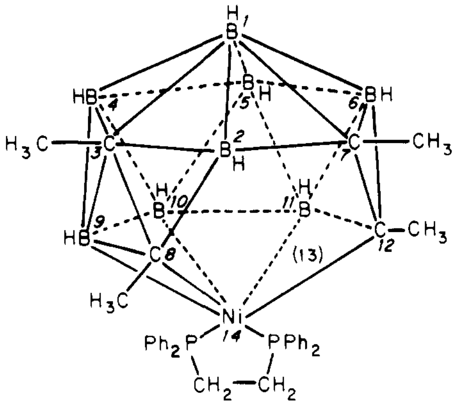
C[19b,55]



D[56]



E[58]



F[18a]

A (1): 2,3-μ-(dimethylphosphino)-*nido*-pentaborane(9)

(2): 2,3-μ-(dimethylphosphino)-(2,3-μH),(2,5-μH),(3,4-μH),(4,5-μH)-6-debor[O_h-(141)-Δ^8-*closo*]hexaborane(9)

B: 8-(η^5-cyclopentadienyl)-2,3,4,5-tetraphenyl-2,3,4,5-tetracarba-8-cobalta-1-debor[C_{2v}-($1v^6 4v^4 22$)-Δ^{14}-*closo*]nonaborane(7)

C: 5,8-bis(η^5-cyclopentadienyl)-2,4-dimethyl-(3,6-μH),(3,7-μH)-2,4-dicarba-5,8-dicobalta-1-debor[C_{2v}-($1v^6 2v^4 422$)-Δ^{18}-*closo*]undecaborane(10)

D: 1,1-bis(triphenylphosphine)-(5,11-μH)-6,12-dicarba-1-argenta-2,9-didebor[C_{2v}-($1v^4 22v^6 422$)-Δ^{22}-*closo*]tridecaborane(11) (the locant set 9,2 is higher than 8,3[57])

E: 9-hydrido-9,10-bis(triethylphosphine)[10-dehydro-7,8-dicarba-9-platina-12-debor[I_h-(1551)-Δ^{20}-*closo*]dodecaborane](9)

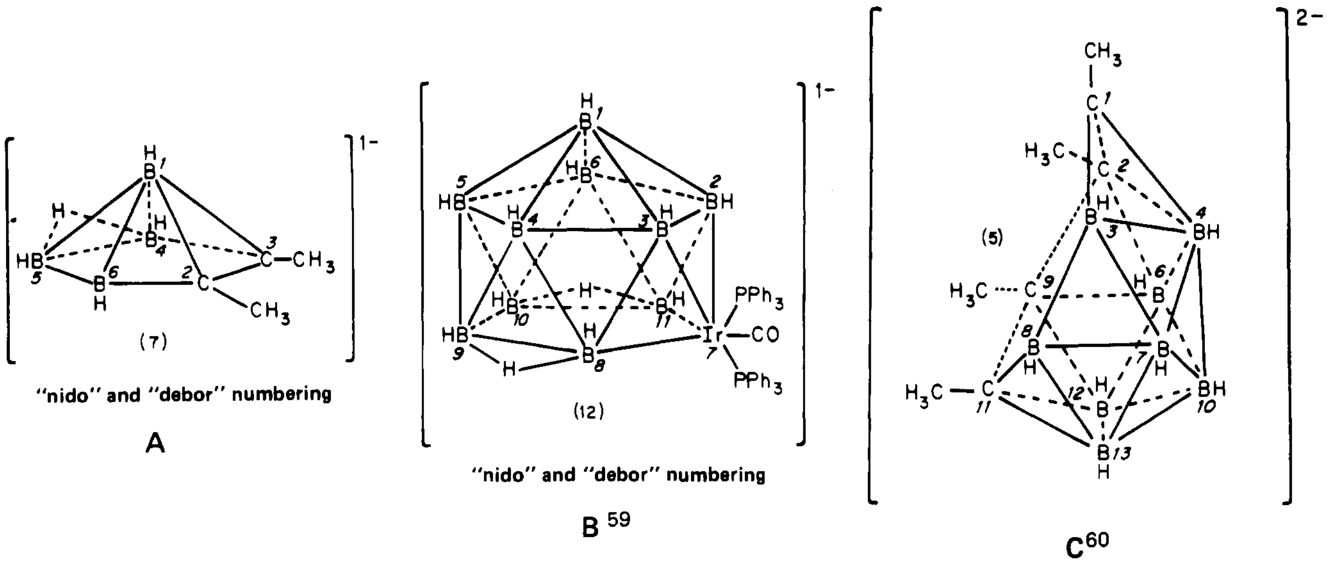
F: 14-[ethylenebis(diphenylphosphine)-P,P']-3,7,8,12-tetramethyl-3,7,8,12-tetracarba-14-nickela-13-debor[D_{6d}-($1v^6 661v^6$)-Δ^{24}-*closo*]-tetradecaborane(12)

Figure 6. Nonclosed polyborane and heteropolyborane derivatives.[51]

of such an approach is that the actual nonclosed polyboron hydride contains fewer skeletal atoms than are in the parent closed polyboron hydride structure. For example, the name 12-debor[I_h-(1551)-Δ^{20}-*closo*]dodecaborate(2−) describes an 11-vertex polyboron anion derived from the closed 12-vertex icosahedral polyboron structure clearly indicated by the descriptor and the numerical prefix dodeca. This operation should be contrasted with a name based on the *nido* system for such an anion, namely, *nido*-undecaborate(2−), where the number of boron atoms in the actual anion is stated. The same problem was discussed in the preceding paper[2a] from an additive viewpoint for capped polyhedral structures.

The concept of subtractive nomenclature is not new.[47c] The subtractive prefix "nor"[47d] has been used for a long time to indicate removal of methylene groups from chains or rings of parent hydrides with trivial or semisystematic names and has been particularly useful in naming natural products such as steroids and terpenes. For example, the name 18-norandrostane describes a structure derived by removal of a methylene group from the methyl group numbered as 18 in the steroid known as androstane. However, it is not nearly as obvious in such a name that the number of skeletal atoms in the actual compound is less than the number in the parent structure as it is in "debor" names of polyboron hydrides, where the number of boron atoms in the parent closed structure is explicitly given by a numerical prefix. Thus, it may be quite desirable in naming nonclosed polyboron hydrides to include the removal of polyhedral vertices, i.e., boron atoms, as part of a descriptor that would precede the name that gives the actual number of boron atoms in the skeletal structure of the polyboron hydride.

Therefore, we propose that removal of vertices from a closed polyhedral structure be indicated by additional symbolism added after the term *closo* in the descriptor for the closed polyhedron developed in our earlier reports.[2b,c] The symbolism we suggest consists of an Arabic number equal to the number of vertices removed, preceded by the minus sign to indicate removal and followed by the italic letter *v* standing for vertex, all enclosed in parentheses. The positions of the polyhedron from which vertices have been removed are given by the appropriate locants for these vertices in the parent closed polyhedron; these locants are cited as superscripts outside the parentheses. Multiple locants are separated by a comma. As for the "debor" positions, the numbers indicating removal of vertices should be as high as possible, consistent with the numbering requirements of the closed polyhedron. For example, descriptors for removal of one vertex and two nonadjacent vertices of an icosahedron would be [I_h-(1551)-Δ^{20}-*closo*$(-1v)^{12}$] and [I_h-(1551)-Δ^{20}-*closo*$(-2v)^{6,12}$], respectively. This descriptor method may be compared with the "debor"



"nido" and "debor" numbering

A

"nido" and "debor" numbering

B[59]

C[60]

A (1): 4,5-μ-hydro-tetrahydro-2,3-dimethyl-2,3-dicarba-*nido*-hexaborate(1−)
(2): 4,5-μ-hydro-tetrahydro-2,3-dimethyl-2,3-dicarba-7-debor[D_{5h}-(151)-Δ^{10}-*closo*]heptaborate(1−)
B (1): 7-carbonyl-8,9:10,11-di-μ-hydro-decahydro-7,7-bis(triphenylphosphine)-7-irida-*nido*-undecaborate(1−)
(2): 7-carbonyl-8,9:10,11-di-μ-hydro-decahydro-7,7-bis(triphenylphosphine)-7-irida-12-debor[I_h-(1551)-Δ^{20}-*closo*]dodecaborate(1−)
C: octahydro-1,2,9,11-tetramethyl-1,2,9,11-tetracarba-5-debor[C_{2v}-($1v^4 22v^6 522$)-Δ^{22}-*closo*]tridecaborate(2−)

Figure 7. Nonclosed polyboron and heteropolyboron derivatives.

method for a pentagonal pyramidal structure by citing an appropriate portion of the names for the nonclosed polyboron hydride compounds shown in Figures 4D or 5A as follows: (1) descriptor method, [D_{5h}-(151)-Δ^{10}-*closo*($-1)^7$]hexabor...; (2) debor method, 7-debor[D_{5h}-(151)-Δ^{10}-*closo*]heptabor....

Note particularly that the actual number of boron atoms in the nonclosed structure is given by the numerical prefix only in the descriptor name, as discussed above. Comparisons of descriptor and debor methods for other nonclosed polyboron hydrides in Figures 4–7 and in Figures A–C (supplementary material) are given in Table II (supplementary material).

The format proposed above is analogous to that suggested in the preceding paper[2a] for capped polyhedra. We feel that other symbolisms and formats are possible and encourage suggestions.[61] The descriptor method is very useful in naming polyboron hydrides consisting of two or more polyhedra or polyhedral fragments as will be shown in a later paper.

Adaptation of "Seco" and "Cyclo" for Naming Nonclosed Polyboron Hydrides

In order to name some nonclosed polyboron structures now being reported either by the "debor" method or by the descriptor system proposed above, it is necessary to create some rather unusual closed polyhedral structures. These polyhedra may have little or no symmetry or may contain planes of vertices not directly connected by polyhedral edges, i.e., polyhedra with severely concave surfaces. In such cases, it seems preferable to avoid the artificial creation of a closed polyhedral structure or the addition of rules to deal with polyhedral systems having severely concave surfaces. We suggest that these problems can be largely avoided by adapting the prefixes "seco" and "cyclo" to naming polyboron hydride compounds. These prefixes are used for modifying ring structures in organic nomenclature especially for natural products such as steroids.[62] The prefix "seco" is used to indicate fission of a ring, i.e., removal of a bond,[62a] and the prefix "cyclo" to indicate the formation of a bond.[62b] The prefix "seco" has been introduced recently into a type of polyhedral nomenclature,[63] and the prefix "cyclo" has been suggested[64] for describing structures with a "restricted open face".

We suggest that the prefixes "seco" and "cyclo" be incorporated into nomenclature for nonclosed polyboron hydrides for describing removal (seco) or formation (cyclo) of a polyhedral edge in order to provide even more flexibility in describing nonclosed structures. Heteroatom prefixes are added in front of the seco or cyclo name for the corresponding nonclosed polyboron hydride, just as they are for the debor names of nonclosed heteropolyboron hydrides. Examples illustrating the use of these prefixes are given by the first names (1) in Figure 8; for comparison "debor" (and "descriptor") names (2) are also given. Additional examples may be found in the supplementary material (Figure D).

Coordination Nomenclature[53b] for Metallopolyboron Hydrides

In the preceding paper,[2a] we noted that coordination nomenclature has been used for naming metallopolyboranes by describing a polyboron hydride fragment as a ligand on the metal. We also noted that this method has not been altogether satisfactory because of the lack of adequate structural description for the polyboron hydride ligand. However, by using the principles for describing nonclosed polyboron hydrides, i.e.,

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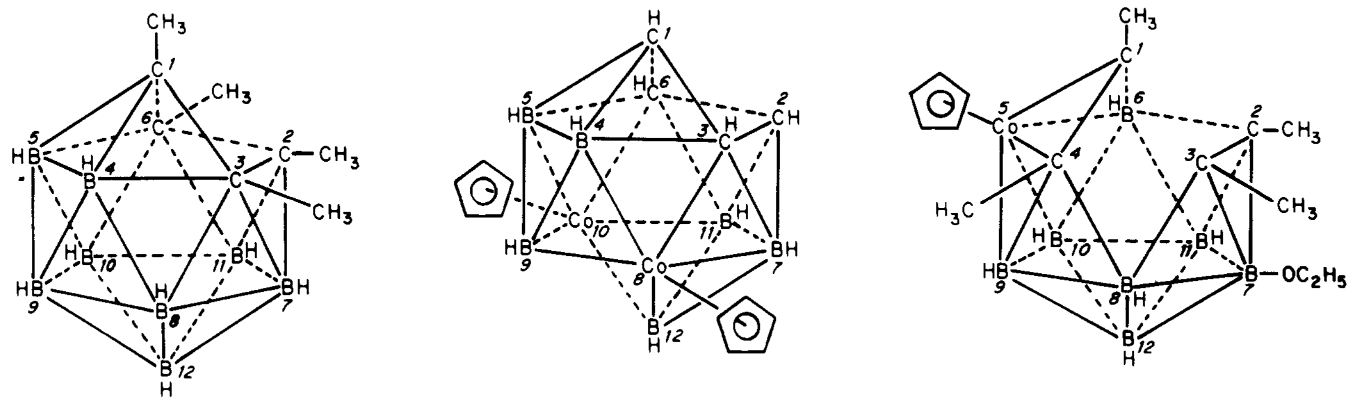
(61) One other symbolism has been proposed (Adams, R. M., private communication) in which the removal of vertices is indicated by the letter "d" followed by the locants of the polyhedron from which the vertices have been removed. We feel that superscript locants are more consistent with other nomenclature principles and that the letter "d" could be easily confused with a common symbolism for indicating isotopic modification by deuterium.

(62) International Union of Pure and Applied Chemistry–International Union of Biochemistry. "Revised Tentative Rules for Nomenclature of Steroids" in "Biochemical Nomenclature and Related Documents", 3rd ed.; International Union of Biochemistry: The Biochemical Society, London, 1978; pp 133–153: (a) Rule 8.1, p 147; (b) Rule 2.4, p 137.

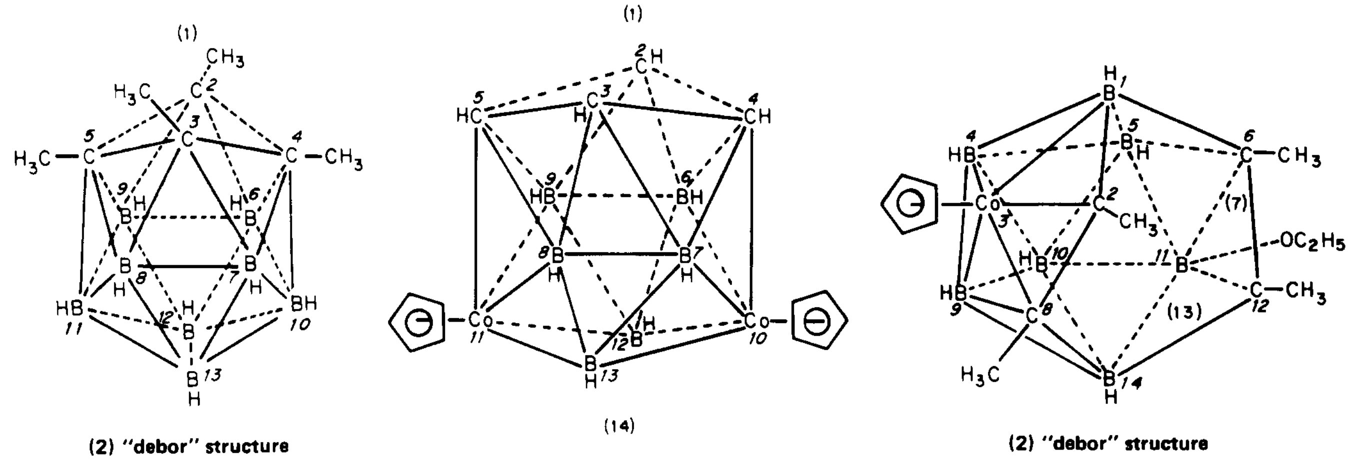
(63) Balogh, D.; Begley, W. J.; Bremner, D.; Wyvratt, M. J.; Paquette, L. A. *J. Am. Chem. Soc.* **1979**, *101* (3), 749–751. Paquette, L. A.; Begley, W. J.; Balogh, D.; Wyvratt, M. J.; Bremner, D. *J. Org. Chem.* **1979**, *44* (21), 3630–3638.

(64) Colquhoun, H. M.; Greenhough, T. J.; Wallbridge, M. G. H.; Heřmånek, S.; Plešek; J. *J. Chem. Soc., Dalton Trans.* **1978**, 944–947.

(65) (a) Pipal, J. R.; Grimes, R. N. *Inorg. Chem.* **1979**, *18* (7), 1936–1940. (b) *J. Am. Chem. Soc.* **1978**, *100* (10), 3083–3088.



(1) "seco" structure (1) "seco" structure (1) "seco" structure



(2) "debor" structure (2) "debor" structure (2) "debor" structure

A^{60} B^{65a} C^{65b}

A (1): 1,2,3,6-tetramethyl-1,2,3,6-tetracarba-1,2-seco[I_h-(1551)-Δ^{20}-*closo*]dodecaborane(12)
(2): 2,3,4,5-tetramethyl-2,3,4,5-tetracarba-1-debor[C_{2v}-($1v^{4}22v^{6}422$)-Δ^{22}-*closo*]tridecaborane(12)
2,3,4,5-tetramethyl-2,3,4,5-tetracarba[C_{2v}-($1v^{4}22v^{6}422$)-Δ^{21}-*closo*$(-1v)^{1}$]dodecaborane(12)
B (1): 8,10-Bis(η^5-cyclopentadienyl)-1,2,3,6-tetracarba-8,10-dicobalta-1,2:9,12-diseco[I_h-(1551)-Δ^{20}-*closo*]dodecaborane(10)
(2): 10,11-bis(η^5-cyclopentadienyl)-2,3,4,5-tetracarba-10,11-dicobalta-1,14-didebor[D_{2h}-($1v^{4}22v^{6}42v^{6}21v^{4}$)-$\Delta^{24}$-*closo*]tetradecaborane(10)
10,11-bis(η^5-cyclopentadienyl)-2,3,4,5-tetracarba-10,11-dicobalta[D_{2h}-($1v^{4}22v^{6}42v^{6}21v^{4}$)-$\Delta^{24}$-*closo*$(-2v)^{1,14}$]dodecaborane(10)
C (1): 5-(η^5-cyclopentadienyl)-7-ethoxy-1,2,3,4-tetramethyl-1,2,3,4-tetracarba-5-cobalta-1,2:1,3:3,4-triseco[I_h-(1551)-Δ^{20}-*closo*]dodecaborane(11)
(2): 3-(η^5-cyclopentadienyl)-11-ethoxy-2,6,8,12-tetramethyl-2,6,8,12-tetracarba-3-cobalta-7,13-didebor[D_{6d}-($1v^{6}661v^{6}$)-Δ^{24}-*closo*]tetradecaborane(11)
3-(η^5-cyclopentadienyl)-11-ethoxy-2,6,8,12-tetramethyl-2,6,8,12-tetracarba-3-cobalta[D_{6d}-($1v^{6}661v^{6}$)-Δ^{24}-*closo*$(-2v)^{7,13}$]dodecaborane(11)

Figure 8. "Seco" and/or "cyclo" names for nonclosed heteropolyboron hydrides.[51]

polyhedral fragments, as given in this report, coordination nomenclature can provide structurally definitive names for many metallopolyboron hydrides.

At the present time, coordination names are unambiguous only when one metal atom is treated as the central atom, or coordination center. Two or more metal atoms can be treated as coordination centers only if the polyboron hydride polyhedral fragment is completely symmetrical itself and symmetrical with respect to the di- or polynuclear coordination center. This is necessary because methods for indicating specific central atoms to which a ligand, or part of a ligand, is attached have not yet been developed.

Although ligand names for polyboron hydride fragments can be derived from neutral polyborane names by the removal of an appropriate number of hydrogen atoms, it seems much more appropriate to generate such ligand names on the basis of anionic polyboron hydride fragments. For example, the closed metallopolyboron hydride shown as Figure 5E in the preceding paper[2a] (and as Figure E-I in the supplementary material to this paper) would be named by current principles of coordination nomenclature as follows: hydrido[(5,6,7,8,9,10-η)-nonahydro-9-(triphenylphosphine)-5,6-dicarba-*nido*-decaborato(2−)]bis(triphenylphosphine)ruthenium.[66] (The numbering for this ligand name is shown by Figure E-I(1) in the supplementary material to this paper.) Other examples of coordination nomenclature for closed metallopolyboron hydrides are given in the supplementary material (Figures E and F).

Nonclosed metallopolyboron hydride structures can also be named by coordination nomenclature. Coordination names for some of the nonclosed monometallopolyboron hydride structures shown in various figures of this report and supplements are given in Table III (supplementary material). Numberings for the nonclosed polyboron hydride ligands used

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(66) Descriptor and debor names: hydrido[(2,3,4,5,6,7-η)nonahydro-3-(triphenylphosphine)-2,4-dicarba[C_{2v}-($1v^{6}2v^{4}422$)-Δ^{18}-*closo*$(-1v)^{1}$]-decaborato(2−)]bis(triphenylphosphine)ruthenium *and* hydrido-[(2,3,4,5,6,7-η)nonahydro-3-(triphenylphosphine)-2,4-dicarba-1-debor-[C_{2v}-($1v^{6}2v^{4}422$)-Δ^{18}-*closo*]undecaborato(2−)]bis(triphenylphosphine)-ruthenium, respectively.

in these names are shown in Figure G (supplementary material). Further development of principles for naming di- and polynuclear coordination systems would permit naming more complex metallopolyboron hydrides by coordination nomenclature.[67]

Choice of System

In this report, and in the preceding paper,[2a] we have suggested several methods for describing both closed and nonclosed polyboron hydride structures and their hetero analogues (including metallo analogues). In many cases, two or more systems can be applied in naming the same polyboron hydride structure, even if we discount relatively minor variations within a system. For example, a closed metallopolyborane may be named on the basis of a parent polyborane using replacement prefixes, or it may be named by coordination nomenclature. A nonclosed metallopolyborane may be described by *nido* or *arachno* prefixes (where appropriate), by the "debor" method, by using a seco or cyclo prefix, or even by coordination nomenclature.

It has not been our purpose in these reports to recommend a preference for one system or another. Authors will certainly establish preferences as needed for different purposes. It has been our intent to introduce methods for describing unambiguous, structurally definitive names, not necessarily unique names.

Summary

In this report we have applied the methods for naming closed polyboron hydride systems developed in the preceding paper[2a] to nonclosed polyboron hydride systems, their hetero (including metallo) analogues, and derivatives. (1) We have suggested that the familiar descriptive prefixes *nido*- and *arachno*- can be used to describe certain nonclosed polyboron hydride structures, while at the same time caution was expressed about extended usage of these prefixes. (2) The "debor" method, briefly introduced into nomenclature rules for polyboron hydride systems,[3a] has been developed and applied in naming many nonclosed polyboron hydride structures. (3) The principles of the descriptor system for describing capped polyhedral systems developed in our earlier report[2a] have been extended to naming polyhedral fragments. (4) We have suggested that the prefixes "seco" and "cyclo", used to great advantage in organic nomenclature, be adapted for naming nonclosed polyboron hydride structures, especially where the debor system would require the creation of unusual closed polyhedral structures. (5) Finally, we have applied the principles described for nonclosed polyboron hydrides in naming metallopolyboron hydrides by coordination nomenclature.

Supplementary Material Available: Tables I–III, listing "debor" names for *nido*- and *arachno*-polyboron hydrides, "debor" and "descriptor" names for nonclosed polyboron hydrides, and "coordination" names for some nonclosed monometallopolyboron hydrides, Figures A–F, showing additional structures and names for nonclosed polyboron and heteropolyboron hydrides and closed metallopolyboron hydrides, and Figure G, showing ligand numberings for coordination names in Table III (12 pages). Ordering information is given on any current masthead page.

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[67] Development of coordination nomenclature for di- and polynuclear coordination systems is under study by various inorganic nomenclature groups.

Contribution from the Laboratoire de Chimie de Coordination du CNRS,
associé à l'Université Paul Sabatier, 31400 Toulouse, France

Coordination Sites of 5-Nitro-6-carboxyuracil: UV Study and X-ray Structure Determination of Diammine(5-nitroorotato)copper(II) Hydrate and Hexaamminebis(5-nitroorotato)tricopper(II) Pentahydrate

PHILIPPE ARRIZABALAGA, PAULE CASTAN,* and FRANÇOISE DAHAN

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A systematic study of UV spectra of 5-nitroorotic acid, for various pH values, shows that in the presence of metal ions (Cu(II)) the ligand is fully deprotonated. Two complexes, $Cu(NH_3)_2(C_5HN_3O_6)\cdot H_2O$ (A) and $Cu_3(NH_3)_6(C_5N_3O_6)_2\cdot 5H_2O$ (B), have been prepared and investigated. Both complexes crystallize in the monoclinic system. Crystal data for A: space group $P2_1/c$, $a = 10.417$ (2) Å, $b = 7.212$ (1) Å, $c = 14.378$ (3) Å, $\beta = 94.30$ (2)°, $V = 1077.2$ Å^3, $Z = 4$, 1806 reflections, $R = 0.036$. Crystal data for B: space group $C2/c$, $a = 18.823$ (3) Å, $b = 7.329$ (1) Å, $c = 20.081$ (6) Å, $\beta = 105.33$ (2)°, $V = 2671.5$ Å^3, $Z = 4$, 2216 reflections, $R = 0.054$. These studies give the first evidence that an orotic acid derivative can coordinate the Cu^{2+} ion simultaneously by the two nitrogen sites of the completely deprotonated ligand.

Introduction

It has been largely demonstrated that orotic acids occupy a rather unique position in being the only effective precursor in the biosynthesis of pyrimidine bases of nucleic acids in living organisms. It is now established that during these processes the presence of metal ions is necessary,[1,2] particularly during the phosphoribosylation of orotic acids;[3] one of the roles played by the metal is making orotic acid available in the form of its reactive N(3)H dianion (Figure 1) where N(1) is unsubstituted, thus contributing to phosphoribosylation at the N(1) site. In this view, elucidation of metal ion effects on the pyrimidine nucleus could possibly lead to a better understanding of processes occurring in living systems.

Orotic acid is a potentially polydentate ligand, since coordination may occur through the two nitrogen atoms of the pyrimidine ring, the two carbonylic oxygens, and also the carboxyl group; moreover, the complexity of the pyrimidine system results from effects of pH changes and group substitutions on the ratio of tautomeric forms of HL^{2-}.

With this in mind, metal bonding studies (spectroscopic, potentiometric, etc.) have been carried out in aqueous solutions,[4–10] the determination of the crystal structures of the

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[2] Lieberman, J.; Kornberg, A.; Simms, E. S. *J. Biol. Chem.* **1955**, *215*, 403.

[3] Victor, J.; Greenberg, L. B.; Sloan, D. L. *J. Biol. Chem.* **1979**, *254*, 2647.

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