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Editor's Note.—The release of a large volume of work on boron cage structures created novel problems of nomenclature and symbolism. The editor appealed to Dr. Roy Adams, Chairman, and other members of the Nomenclature Committee of the Inorganic Division of the A.C.S. for help in solving these problems. The report presented here was prepared in response to that appeal. While the recommendations in the report have not been formally approved by nomenclature committees of either the A.C.S. or I.U.P.A.C., the report does summarize the best judgment of a majority of the workers who are deeply concerned with nomenclature in this area. The schemes outlined are recommended for use in this journal until such time as these recommendations are replaced by official A.C.S. or I.U.P.A.C. nomenclature decisions.

R. W. Parry
Editor

Contribution from the Department of Chemistry, Geneva College, Beaver Falls, Pennsylvania

Cage Borane Nomenclature

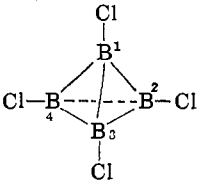
By Roy Adams

Received October 9, 1963

Due to the release of a large volume of information on $B_{10}C_2H_{12}$ and its derivatives, and due to differences in the nomenclatures proposed, a special meeting of the boron nomenclature subcommittee with interested parties was held September 11, 1963, in New York to seek agreement in this area. The following system was agreed upon.

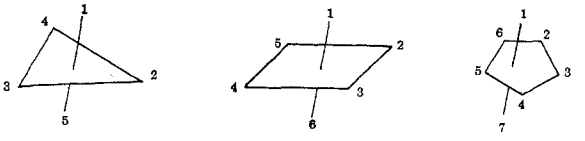
Since several classes of compounds with cage type structures are known (polyphosphates, polysilicates, heteropolyanions, and, in particular, for present purposes, some of the hydropolyborate ions and the dicarbapolyboranes) a generally accepted nomenclature term is needed to indicate such structures. (By a cage structure is meant a closed polyhedron with no bridging hydrogens.) Greek prefixes have been used in the past for such purposes. "Clovo" from the Greek word for cage, "κλωβοσ," has been suggested and was adopted.[1]

As an example, the simplest closed polyhedron is a tetrahedron. The compound B_4Cl_4 has a tetrahedral structure.[2] Tetrachloroclovotetraborane(4) gives more structural information than the binary compound name, tetraboron tetrachloride.

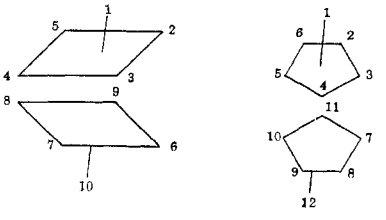


In the cage type polyborane structures the number of hydrogen atoms generally requires a cage structure, hence *the prefix "clovo" may in general practice be useful only to supplement or replace the numerical suffix indicating numbers of hydrogen atoms; e.g.*, the names tetrachlorotetraborane(4) or tetrachloroclovotetraborane also identify this compound.

The problem of the location of substituents has already been raised. The numbering system adopted for a tetrahedron is shown. Beyond a tetrahedral structure the cages may be considered to be bipyramids. In consistency with the numbering in the lower boranes, an apex atom should be numbered first, then the belt or girdle atoms, then the opposite apex.



For icosahedral and similar structures it appears best to number one apex, then the first ring of belt atoms, then the second ring, and finally the opposite apex.

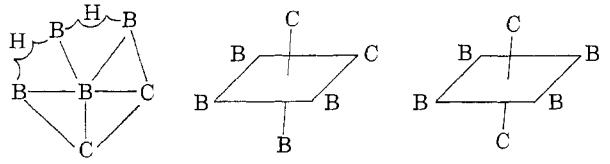


(1) J. Van Wazer, "Phosphorus and Its Compounds," Vol. I, Interscience Publishers, Inc., New York, N. Y., 1958, p. 89.
(2) M. Atoji and W. N. Lipscomb, *J. Chem. Phys.*, **21**, 172 (1953).

This gives closest agreement with the numbering already in use for pentaborane(9) and hexaborane.

The need for the early decision on nomenclature in this area revolved around the use of the term "carborane." This has been used in both generic and specific senses. Different representatives at the meeting had views of the generic meaning ranging from any boron–carbon hydride to clovo boron–carbon hydrides with two skeletal carbon atoms. After considerable discussion, the concensus was that *the term carborane should cover clovo or near-clovo boron–carbon hydrides with skeletal carbon atoms; i.e.*, $B_4C_2H_8$[3] and $B_9C_2H_{13}$[4] should be included as well as predicted compounds such as clovo $B_8C_4H_{12}$,[5] but that the term should not be used to include alkyl-substituted boranes such as ethyldecaborane.

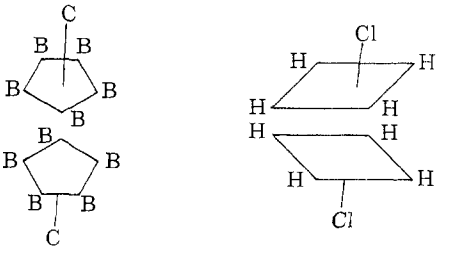
The carboranes reported at present are apparently cage structures with the exception of two. In systematic nomenclature these can conveniently be named by the "oxa, aza" system with the hetero atoms having as low numbers as possible. In the case of the carboranes with four boron atoms, there is evidence for the types shown in Fig. 1. (terminal hydrogens are omitted).



2,3-dicarbahexaborane(8)[3] 1,2-dicarbaclovohexaborane(6)[6] 1,6-dicarbaclovohexaborane(6)[6]

Figure 1.

Other applications of the system include those shown in Fig. 2.



terminal hydrogens are omitted borons are omitted

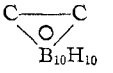
1,12-dicarbaclovododecaborane(12) 1,10-dichlorooctahydroclovodecaborate(2−)

Figure 2.

For the substance dicarbaclovododecaborane(12) two isomers and many derivatives are known with substituents on the carbon atoms. A trivial name is needed. "Carborane" has also been extensively used as this trivial specific name. This should be permissible if clearly defined in an article.

The less common isomer has been called neocarborane. This trivial name was approved until further structural definition. Most workers feel that these isomers are 1,2- and 1,7-dicarbaclovododecaboranes. However, others question these structures. Until definitive studies are available, such substances with substituents on the carbon atoms should be named with (C,C′), if necessary, to locate substituents.

The derivative with an ethyl and a propyl group on the carbon may then be named C-ethyl,C′-propylcarborane. Where necessary carboranyl may be used for the $B_{10}C_2H_{11}$ radical and carboranylene for the $B_{10}C_2H_{10}$ diradical. To represent the latter in formulas, tables, etc., $(B_{10}H_{10}C_2)$ or $(CB_{10}H_{10}C)$ should be adequate. These representations have the advantage of keeping the formulas on one typed line: *e.g.*, $C_2H_5(CB_{10}H_{10}C)C_3H_7$ for the above derivative. For situations when further structural indication is imperative, the symbol



was adopted for use with carborane only.

(3) T. P. Onak, R. E. Williams, and H. G. Weiss, *J. Am. Chem. Soc.*, **84**, 2839 (1962); I. Shapiro and H. G. Weiss, U. S. Patent 3,086,996 (April 23, 1963).

(4) D. Grafstein, *Inorg. Chem.*, in press.

(5) R. E. Williams, private communication.

(6) I. Shapiro, B. Keilin, R. E. Williams, and C. D. Good, *J. Am. Chem. Soc.*, **85**, 3167 (1963).