

addition it has nine close water molecule neighbors, most of which are undoubtedly hydrogen-bonded. No hydrogen bonds link bases directly.

(6) The bond distances and angles do not differ significantly from the expected values; the standard errors average about 0.012 Å. and 0.7° for distances and angles not involving hydrogen atoms. The C₁' atom of each sugar is very nearly in the plane of the base to which it is attached (deviation 0.01 and 0.03 Å.), unlike the situation in adenosine phosphate² and 5-fluoro-2'-deoxy-β-uridine.⁵

(5) D. R. Harris and W. M. Macintyre, unpublished work.

CONTRIBUTION No. 1639
DEPARTMENT OF CHEMISTRY
UNIVERSITY OF CALIFORNIA
LOS ANGELES, CALIFORNIA

ELI SHEFTER
MALCOLM BARLOW
ROBERT SPARKS
KENNETH TRUEBLOOD

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Molecular Structure of a Carborane (1,2-Dicarboclovododecaborane) Derivative, B₁₀Cl₈H₂C₂H₂

Sir:

The carborane^{1,2} B₁₀C₂H₁₂ is usually assumed²⁻⁴ to have very nearly the icosahedral geometry of the B₁₂-H₁₂⁻² ion⁵ (Fig. 1a). However, an X-ray diffraction study⁶ of B₁₀H₁₀C₂(CH₂Br)₂ has supported an ethylene decaborane type of B₁₀C₂ unit (Fig. 1b.). We report here the results of a three-dimensional single crystal X-ray diffraction study of B₁₀Cl₈H₂C₂H₂ which indicates the nearly regular icosahedral arrangement for the B₁₀C₂ structural unit (Fig. 1a).

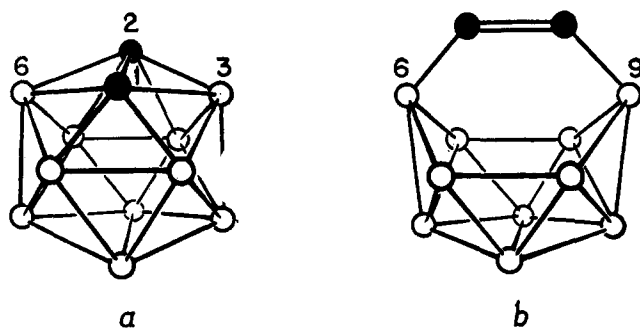


Fig. 1.—a represents the near icosahedral B₁₀C₂ framework in B₁₀Cl₈H₂C₂H₂. Open and black circles indicate, respectively, B atoms and C atoms. Substitution of Cl has taken place at all H atoms of the parent B₁₀C₂H₁₂ except those attached to B₃, B₆, C₁, and C₂. b represents the boron-carbon framework described⁶ for B₁₀H₁₀C₂(CH₂Br)₂.

The crystal symmetry is Pbn_a, and there are eight molecules in a unit cell of dimensions $a = 17.10$, $b = 13.46$, and $c = 13.65$ Å. All B and C atoms were located and distinguished from one another by their electron densities in three-dimensional Fourier series

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(3) R. Hoffmann and W. N. Lipscomb, *J. Chem. Phys.*, **36**, 3489 (1962); *Inorg. Chem.*, **2**, 231 (1963).

(4) W. N. Lipscomb, "Boron Hydrides," The W. A. Benjamin Co., New York, N. Y., 1963.

(5) J. Wunderlich and W. N. Lipscomb, *J. Am. Chem. Soc.*, **82**, 4427 (1960).

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from which the Cl atoms had been subtracted. The present value of $R = \frac{\sum |F_o| - |F_c|}{\sum |F_o|}$ is 0.13 for the 1739 observed X-ray diffraction maxima.

Two other features of the structure are of interest here. The C-C distance of 1.68 ± 0.02 Å. is considerably larger than the distance⁷ of 1.43 Å. in B₄H₆C₂(CH₃)₂, which contains two adjacent C atoms in a slightly less strongly electron-deficient environment. Also, substitution of Cl has taken place at all B atoms (4,5,7,8,9,10,11,12) except for the two B atoms (3,6) which are indicated to be most positively charged by both molecular orbital and resonance theories³ of charge distribution.

A comparison⁸ of ¹¹B nuclear magnetic resonance in B₁₀C₂H₁₂ and in B₁₀Cl₁₀C₂H₂ indicates that direct chlorination produces essentially no change in the B₁₀C₂ framework. Also, the thermal stability of carborane up to a temperature of 470°, at which it transforms³ readily and without decomposition to neocarborane,^{8,9} is more easily understood on the basis of the icosahedral structure (Fig. 1a) rather than the ethylene decaborane type of structure (Fig. 1b). However, the possibility that the structure of Fig. 1b is an intermediate in the synthesis of carborane derivatives is not excluded. Further structural studies of carborane and neocarborane derivatives are in progress.

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DEPARTMENT OF CHEMISTRY
HARVARD UNIVERSITY
CAMBRIDGE 38, MASSACHUSETTS

JOSEPH A. POTENZA
WILLIAM N. LIPSCOMB

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Decreasing Sorption Effect with Increasing Pressure

Sir:

In a recent article by Cimino, *et al.*,¹ the hypothesis was advanced that the surface of polycrystalline ZnO was very likely conditioned for further H₂ uptake by a rapid initial adsorption of H₂. This initial adsorption is frequently observed^{2,3} with other systems but much less frequently measured. A somewhat similar effect has been observed during the study of the uptake of oxygen by Pr₂O₃. This effect, in general, is a small loss of sorbed gas with an increase in gas pressure. The effect has been noted during "equilibrium" as well as kinetic measurements. Three separate pieces of evidence seem to indicate that the effect is real.

(1) During the course of a general study of the Pr-O system it was noted that in some cases the oxygen content on and/or in the solid PrO_x could be reduced slightly by increasing the oxygen pressure. The effect was observed specifically⁴ during the investigation of

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