We are indebted to Professor H. I. Schlesinger and Dr. I. Shapiro for samples of pentaborane and to the Office of Naval Research (Contract N6onr 24423) for support during most of this investigation.

CHEMISTRY DEPARTMENT   KENNETH HEDBERG
CALIFORNIA INSTITUTE OF TECHNOLOGY MORTON E. JONES
PASADENA 4, CALIFORNIA   VERNER SCHOMAKER
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THE MOLECULAR STRUCTURE OF PENTABORANE

Sir:

If one compares the recently-determined structures of boron carbide[1] and decaborane[2] on the one hand with the structure of calcium boride[3] and possible structures of pentaborane on the other, the most reasonable structure of B_5H_9 (M. V. King and W. N. Lipscomb, unpublished) that can now be predicted is a tetragonal pyramid of molecular symmetry C_{4v}, such as that shown in Fig. 1. Apparently a molecule of this structure was overlooked in the earlier electron diffraction study,[4] because a recent study by Hedberg, Jones and Schomaker[5] shows that the electron diffraction pattern is consistent with such a model, but is also not inconsistent with some quite different, but chemically less reasonable, models.

We have completed an X-ray diffraction study of single crystals of pentaborane. The crystals are pyroelectric, and belong to the tetragonal space group C_{4v}^9–I4mm., with two molecules in a unit cell of dimensions $a = 7.16$ Å. and $c = 5.38$ A. Evaluation of parameters from three-dimensional sections leads to the values:

B_2–B_2 = 1.77 ± 0.02 Å. H_3...H_3 = 1.95 ± 0.09 A.
B_1–B_2 = 1.66 ± 0.02 Å. $\angle$ B_1,B_2, H_3 = 115 ± 5°
B_1–H_1 = 1.21 ± 0.05 Å.   External dihedral angle be-
B_2–H_2 = 1.20 ± 0.07 Å.   tween planes $B_1B_2B_2$ and
B_2–H_3 = 1.35 ± 0.04 Å. $B_2B_2H_3$ = 190 ± 5°

As in decaborane the intermolecular approaches are all between hydrogen atoms. These approaches range from 2.46 to 2.96 Å. which appear reasonable in view of the very large temperature factor in the crystal. The diagonal of the base of the pyramid has the direction of the a axis. It may be noted that the average boron-boron distance in the molecule is apparently about two per cent. smaller in the solid state than in the gaseous state, a situation previously observed only in hexamethylenetetramine.[6]

The interatomic binding in pentaborane, which is similar to decaborane, is of the 'metallic' type and in such a case we may expect Pauling's relation[7] $r = $

(1) G. S. Zhdanov and N. G. Sevast'yanov, *Compt. rend. acad. sci. U.S.S.R.*, **32**, 432 (1941); H. K. Clark and J. L. Hoard, THIS JOURNAL, **65**, 2115 (1943).

(2) J. S. Kasper, C. M. Lucht, and D. Harker, *Acta Cryst.* **4**, 436 (1950).

(3) L. Pauling and S. Weinbaum, *Z. Krist.*, **87**, 181 (1934).

(4) S. H. Bauer and L. Pauling, THIS JOURNAL, **58**, 2403 (1936).

(5) K. Hedberg, M. Jones, and V. Schomaker, private communication. A preliminary report on this determination was made at the Chicago meeting of the American Chemical Society, September, 1950. We are indebted to these authors for making available to us their results, described in the preceding letter.

(6) V. Schomaker and P. A. Shaffer, Jr., THIS JOURNAL, **69**, 1555 (1947); P. A. Shaffer, Jr., *ibid.*, **69**, 1557 (1947).

(7) L. Pauling, THIS JOURNAL, **69**, 542 (1947). The details of the present method of applying Pauling's relation were suggested to us by K. Hedberg and V. Schomaker. Following their suggestion also we
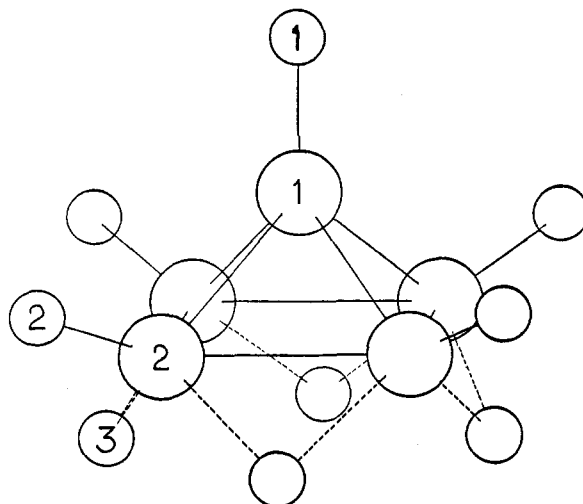
Fig. 1.—The pentaborane molecule: boron and hydrogen atoms are represented by large and small circles, respectively.

$r_1 - 0.3 \log n$ to be reasonably valid. If we choose a covalent radius for hydrogen equal to 0.36 Å., then the total bond order for the molecule, which should be twelve, will depend upon the choice of the boron single-bond radius. A value of 0.78 Å. for this boron radius satisfies these conditions, thus leading to a total bond order of 12.03. The individual bond orders are $n_{12} = 0.681$, $n_{22} = 0.447$, $n'_{11} = 0.764$, $n'_{22} = 0.794$ and $n'_{23} = 0.447$, where the prime refers to B–H bonds. These orders suggest that the hydrogen atoms are somewhat positively charged and the boron atoms are somewhat negatively charged. This distribution of charge indicates a dipole moment of about 0.6 Debye. Similar calculations lead to a single-bond radius for boron of 0.79 Å. from the diborane molecule, and of 0.81 Å. from the decaborane molecule.

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SCHOOL OF CHEMISTRY   WILLIAM J. DULMAGE
UNIVERSITY OF MINNESOTA   WILLIAM N. LIPSCOMB
MINNEAPOLIS 14, MINNESOTA
             RECEIVED JUNE 5, 1951

PHOTOGRAPHY IN ELECTROPHORESIS OF HEMO-LYZED SERA

Sir:

The occasional necessity for the examination by electrophoresis of hemolyzed sera, or of solutions of hemoglobin or other proteins having high optical density except for red or infrared light, has presented a technical problem in photography. The customarily used mercury vapor arc lamp has strong green and yellow lines, but its red intensity