ON THE STRUCTURE OF TETRABORANE

Sir:

We have reinvestigated gaseous tetraborane by electron diffraction. The butane-like model with tetrahedral bond angles as reported by Bauer[1] is incompatible with our data; values of $\angle$B–B–B = 90° and $\angle$B–B–H = 133.5° do bring it into agreement, but the latter angle is out of the question, especially for the "methylenic" hydrogen atoms. No exhaustive investigation of the butane-like structure was attempted, however, because a structure (Fig. 1) plausibly related to the known boron hydride structures[2] was discovered and shown
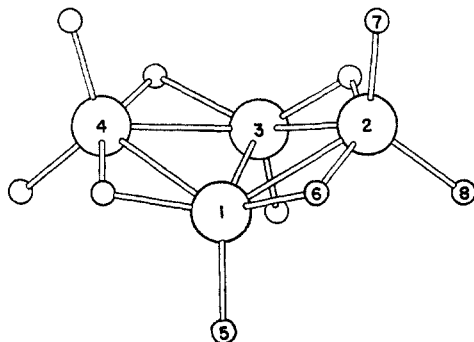

Fig. 1.—The B_4H_{10} structure.

to be in excellent agreement with the diffraction pattern early in our work,[3,4] and has since been
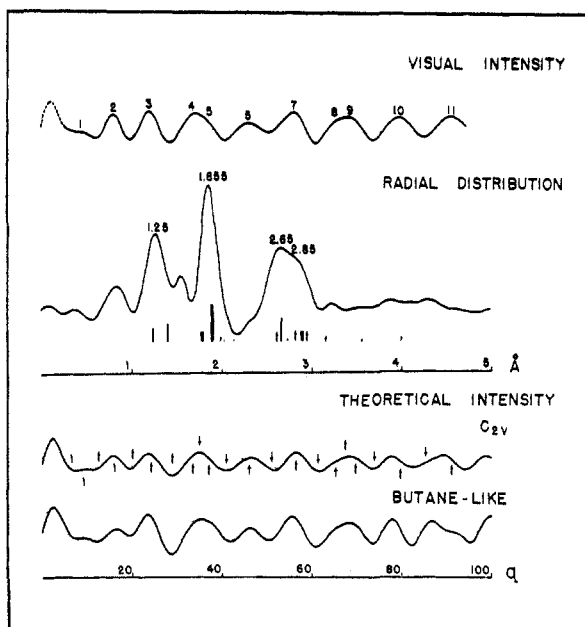

Fig. 2.—Visual, radial distribution and theoretical intensity curves. The theoretical intensity curves are for the butane-like model with $\angle$ B–B–B = 90° and $\angle$ B–B–H = 133.5° and for the C_{2v} model described in the text.

(1) S. H. Bauer, THIS JOURNAL, **60**, 805 (1938).

(2) For references and discussion see K. Hedberg, M. E. Jones, and V. Schomaker, *Proc. Nat. Acad. Sci. U. S.*, **38**, 679 (1952).

(3) K. Hedberg, V. Schomaker and M. E. Jones, Paper E.D. 17, Second International Congress of Crystallography, Stockholm, June 2T–July 5, 1951. The structure, although not mentioned in the Abstract, was presented at the meeting.

(4) Quarterly Progress Report, October 23, 1951, Contract N6onr 24423.

established by Nordman and Lipscomb by the crystal structure investigation reported in the following Communication. The atomic arrangement is closely similar to that of the apical groups in decaborane and is comparable to the arrangements in diborane and stable pentaborane.

Approximate values for the numerous parameters of the C_{2v} model are

B_1–B_2 = 1.85 Å., B_1–B_3 = 1.76 Å.

$B_2 \cdots B_4$ = 2.88 Å. (Dihedral $\angle B_1B_3B_4$–$B_1B_3B_2$ = 124°32′)

B_1–H_5 = B_2–H_7 = B_2H_8 = 1.19 Å.

B_2–H_6 = 1.33 Å., B_1–H_6 = 1.43 Å., H_6 in plane of $B_1B_2B_3$

$\angle B_3$–B_1–H_5 = 118°20′ and $\angle B_{1,3}$–B_2–$H_{7,8}$ = 117°6′

These values were obtained primarily from the radial distribution curve (Fig. 2); they were refined by a (necessarily incomplete) correlation treatment. The H_6 parameters are highly uncertain, but the B–H distance 1.19 Å. and the B–B bond distances warrant comparison with the crystal values.

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CONTRIBUTION NO. 1828

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THE MOLECULAR STRUCTURE OF B_4H_{10}

Sir:

As a result of a complete analysis of 616 observed reflections from a single crystal of B_4H_{10}, we have determined the molecular structure. There are four molecules in a monoclinic unit cell having parameters a = 8.68, b = 10.14, c = 5.78Å. and β = 105.9°. The space group $P2_1/n$ is unambiguous, and the twelve independent positional parameters of the boron atoms were determined from three-dimensional Fourier analysis. The hydrogen atoms were readily observable, and were also located more precisely from a three-dimensional Fourier series from which the boron atoms had been subtracted.

The molecular structure of B_4H_{10} is shown in Fig. 1. No molecular symmetry elements are required by the space group of the crystal, but the molecular dimensions indicate that the symmetry of the isolated molecule is C_{2v}. For brevity, we
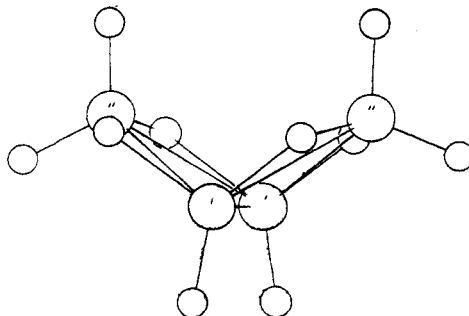

Fig. 1.—The molecular structure of B_4H_{10}.