MOLECULAR STRUCTURE OF $B_{10}H_{12}(CH_3CN)_2$

Sir:

Decaborane reacts with acetonitrile to form[1] a substitution derivative, $B_{10}H_{12}(CH_3CN)_2$, in which a covalent bond has been tentatively assumed[1] between the CH_3CN groups. On the other hand, our results indicate, somewhat surprisingly, that the CH_3CN groups are linear and are each attached by a single N–B bond, and that they are not attached to each other.

The molecular structure, shown in Fig. 1, is based on the boron arrangement in decaborane. The heavy atoms were located from the Patterson function calculated from 956 X-ray diffraction maxima obtained from a single crystal. The hydrogen atom positions, except for those of the methyl groups, were uniquely established from difference electron density maps.

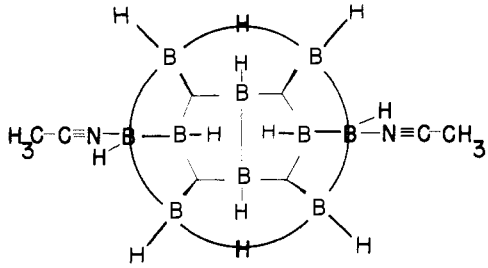

Fig. 1.—Topological drawing of the $B_{10}H_{12}(CH_3CN)_2$ structure showing the three-center bond approximation to the valence theory. The isolated molecule apparently has C_{2v} symmetry, which has been distorted here for clarity in the case of two hydrogen atoms. Regarded as a derivative of $B_{10}H_{14}^{-2}$, the boron-hydrogen arrangement has the 2632 topology,[3] with two bridge hydrogen atoms. Bond distances are within normal ranges.

Unit cell values are $a = 7.81$, $b = 11.31$, $c = 14.18$ and $\beta = 96°52'$. The space group of I2/c requires that the molecule shall have at least a twofold axis. Refinement, still in progress, has reached the values of $R = \Sigma||F_0| - |F_c||/\Sigma|F_0| = 0.17$ and $r = \Sigma w(F_0^2 - F_c^2)^2/\Sigma w F_0^4 = 0.20$ for all observed reflections.

The structure has interesting chemical implications. First, it is to be regarded as a substitution derivative of $B_{10}H_{14}^{-2}$, not of $B_{10}H_{14}$. This ion has been suggested on the basis of valence theory[2]; its negative charge probably can best be accommodated by transformation from the 4450 topology[2] to either the 2632 or 0814 structures.[3] Second, it suggests that these two particular boron atoms (Fig. 1), presumably most positive in $B_{10}H_{14}$ because of abstraction of negative charge by the two bridge hydrogens, are most susceptible to substitutional attack by an electron donor.

We wish to thank Professor Riley Schaeffer for supplying us with single crystals. We are greatly indebted to Dr. F. L. Hirshfeld, who took many of the diffraction photographs. For financial support we wish to thank the Office of Naval Research, the Office of Ordnance Research and the Shell Development Company. The fourteen hours of computing time on the UNIVAC SCIENTIFIC 1103 were contributed in part by the University of Minnesota.

SCHOOL OF CHEMISTRY JOSINA VAN DER MAAS REDDY
UNIVERSITY OF MINNESOTA WILLIAM N. LIPSCOMB
MINNEAPOLIS 14, MINNESOTA

RECEIVED DECEMBER 10, 1958

(1) R. Schaeffer, THIS JOURNAL, **79**, 1006 (1957).

(2) W. N. Lipscomb, *J. Phys. Chem.*, **62**, 381 (1958). See also R. H. Toeniskoetter, G. W. Schaeffer, E. C. Evers and G. E. Bagley, Abstracts of 134th Meeting, A.C.S., Chicago, Ill., Sept. 7–12, 1958, p. 23–4.

(3) W. N. Lipscomb, Advances in Inorganic and Radiochemistry, Academic Press, Inc., New York, N. Y., Vol. I, 1959, p. 146.

THE ENZYMATIC CONVERSION OF MEVALONIC ACID-2-C^{14} TO AN OLEFINIC ACID[1]

Sir:

Although 3,5-dihydroxy-3-methylpentanoic acid (mevalonic acid, MVA) has been demonstrated to be a very efficient precursor of squalene[2,3] and cholesterol[4] in animal tissues, the identity of dimeric or trimeric intermediates between mevalonic acid and squalene has not been elucidated. We now wish to report the isolation and probable structure of a long-chain olefinic acid which accumulates as a metabolite of MVA in rat liver.

As shown in Table I, the conversion of MVA-2-C^{14} to non-saponifiable lipids requires both the high speed supernatant fraction of rat liver and the microsomes. The omission of microsomes leads to the accumulation of a petroleum ether extractable C^{14}-labeled olefinic acid. The cofactor requirements for both of these conversions were found to be quite similar. Therefore, it seems reasonable to suppose that the long-chain olefinic acid is either an intermediate in squalene biosynthesis or is closely related structurally to an intermediate.

TABLE I

THE INCORPORATION OF MEVALONIC ACID-2-C^{14} INTO AN OLEFINIC ACID

	Total c./m. in acidic fraction	Total c./m. in non-acidic fraction	Total c./m. in non-saponifiable lipid
Soluble enzyme preparation[a]	1140	183	
Soluble enzyme preparation plus microsomes	30		1010

[a] The soluble enzyme preparation consisted of the supernatant fraction after the centrifugation of a rat liver homogenate at 78,410 × *g* for two hours.

A large-scale incubation of MVA-2-C^{14} (S.A. 3,378 c./m./mg.) with the soluble enzyme preparation led to the isolation of 5 mg. of the unsaturated acid (S.A. 5,353 c./m./mg.). The greater specific activity of the unsaturated acid as compared with the original MVA would indicate that MVA was the sole precursor and that it was converted in a net manner with a loss of some portion of the MVA molecule during conversion. The equivalent weight of this acid was found to be 292. Both the specific activity and the equivalent weight would indicate that the acid was only 90% pure based on the proposed structure presented later.[5]

(1) This work was supported by grants from the U. S. Public Health Service and the Nutrition Foundation, Inc.

(2) J. W. Cornforth, R. H. Cornforth, G. Popjak and I. Youhotsky-Gore, *Biochem. J.*, **66**, 10P (1957).

(3) F. Dituri, S. Gurin and J. L. Rabinowitz, THIS JOURNAL, **79**, 2650 (1957).

(4) P. A. Tavormina, M. H. Gibbs and J. W. Huff, *ibid.*, **78**, 4498 (1956).

(5) See J. W. Ogilvie, Jr., THIS JOURNAL, **81**, 756 (1959).