The Cage Compound $(BMe)_6(CH)_4$

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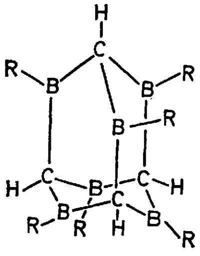
Summary Sealed-tube pyrolysis of BMe_3 permits isolation of the compound $(BMe)_6(CH)_4$ in 25% yield; n.m.r. evidence shows six equivalent BMe and four equivalent CH groups, and an adamantane-like structure is proposed for the boron–carbon cage.

WE recently reported[1] the compound $(BMe)_6(CH)_4$ as one of the components of the complex mixture of products formed in low yield when trimethylborane is thermally decomposed in a flow system. We now find this component to be the major product (25% yield based on starting material consumed) when BMe_3 is decomposed in sealed tubes (1—2 h at 450 °C). Such a high yield is remarkable for a reaction of this type. The compound, a colourless crystalline solid, m.p. 85 °C, is air-sensitive but water-stable and complexes weakly and reversibly with NMe_3 and PMe_2Ph. It is probably identical with a compound of similar physical properties, obtained by previous workers[2] in 4% yield, but assigned the composition $(MeBCH_2)_4$.

The ^1H n.m.r. spectrum of a $(CD_3)_2CO$ solution consists of just two singlets δ (60 MHz, Me_4Si internal reference) 0·57 (18H, BMe) and 3·98 (4H,CH) and the ^{11}B spectrum of just one, fairly broad resonance, δ (28·9 MHz, BF_3,OEt_2 external reference) −63·2. Spectra (^1H and ^{11}B) of the melt and of benzene solutions are similar. The ^{13}C spectrum obtained from the melt was poor in quality but showed two broad and irregularly shaped bands, δ (25·2 MHz, Me_4Si reference) −11·6 (BMe) and −82·2 (CH).

We previously suggested[1] that this compound was the *B*-permethyl derivative of an unknown but predicted[3] *nido*-carborane $B_6H_6C_4H_4$, having a framework based on the B_{10} cage of decaborane. Such a structure may now be excluded since neither the six BMe nor the four CH groups could be equivalent however they might be placed within this carborane framework. The only possible structure having six equivalent boron and four equivalent carbon atoms appears to be one in which the carbon atoms are placed at the corners of a tetrahedron and the boron atoms are placed above each edge of this tetrahedron. This gives an adamantane-like structure shown, the bonding in which may then be readily explained in terms of 2-electron B–C bonds as in organo-boranes, although the possibility of electron-deficient delocalised bonding cannot be entirely discounted. The magnitude of the ^{11}B shift (δ −63·2) seems to support an organoborane type of structure since shifts for a variety of trialkyl- and triaryl-boranes[4] fall between *ca.* −55 and −86·3 (the latter value for BMe_3), whereas the ^{11}B resonances of methyl-substituted B atoms in carboranes[4] fall between *ca.* +20 and −20 (all measured from BF_3,OEt_2).



R = Me

This boron–carbon cage compound appears to be unique in having a stoicheiometry expected of a carborane and yet not possessing the usual carborane type of structure. Its mode of formation, however, resembles that of sila-adamantanes[5] obtained in very much lower yields from the pyrolysis of Me_4Si, although here the Si atoms are in the bridgehead positions. A similar aluminium–carbon cage has been proposed[6] for a compound $(AlMe)_6(CMe)_4$ obtained from a reaction involving Al_2Me_6, although structural evidence is lacking.

A full *X*-ray structural determination is being conducted by Dr. H. Shearer of Durham University. We thank Mr. J. W. Akitt of Leeds University and Dr. R. D. Lapper of Liverpool University, for n.m.r. spectra, and the S.R.C. for support.

(*Received, 8th June* 1973, *Com.* 819.)

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