are presumably responsible for reversing this situation, as we have already suggested.[8]

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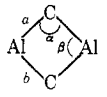
The Molecular Structure and Bonding in Hexamethyldialuminum

Sir:

In the past few months a lively controversy has developed over the nature of the methyl bridge bonding in $Al_2(CH_3)_6$. This author wishes to point out that *on the basis of the published structural data there is no basis for controversy.* Disputation has been engendered solely by incomplete analysis of the available data.

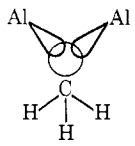
In 1967 Vranka and Amma[1] carried out an X-ray structural study of crystalline $Al_2(CH_3)_6$. They found the distances and angles shown in I and concluded that each bridge bond could best be understood as a two-



$a = b = 2.14 \pm 0.01$ Å
$\alpha = 74.7°$
$\beta = 105.3°$

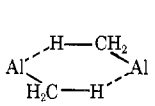
I

electron, three-center (2e-3c) interaction employing an orbital on each Al atom and a quasi-tetrahedral orbital on the carbon atom as previously proposed by Longuet-Higgins[2] and depicted schematically in II.

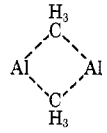


II

More recently, Byram, *et al.*,[3] have claimed that their further refinement of the structure, using Vranka and Amma's own data, led to the conclusions that (a) the Al and C positions as given by Vranka and Amma are correct, but (b) one of the hydrogen atoms of the bridging methyl group is located in or near the central Al–C–Al–C ring plane at distances of 1.08 (12) Å from C and 1.78 (13) Å from Al, the figures in parentheses being the (rather large) estimated standard deviations for these distances. From this they concluded that the structure contains two two-electron hydrogen bridge bonds, such as might be represented by III. Dewar and Patterson[4] have recently depicted structures III and



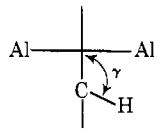
III



IV

IV (which is simply a schematic representation of Vranka and Amma's structure) as alternatives and reported nqr data which they believe favors IV.

When the available structural information is considered *in full*, one finds that III does not depict a viable structural alternative to IV. It is simply an unjustified, incorrect, and misleading drawing. From the C–H and H···Al distances given by Byram, *et al.*, and the *essentially equal* pair of Al–C distances,[5] simple trigonometry shows that the angle γ in V is 93° with an uncertainty of at least 12° due to the esd's of the C–H and H···Al distances. This is entirely compatible with the 2e-3c Al–C–Al bonding situation symbolized



V

by IV and does not require the acceptance of the situation represented by III. The only justifiable conclusion would seem to be that rotation of the bridging methyl groups in IV about their threefold axes may be somewhat restricted with a preference for the rotamer having one H atom in the central ring plane.

In conclusion, the work of Byram, *et al.*, does not, contrary to their claim, raise any real question about the previously accepted view of the structure and bonding of the bridge system in $Al_2(CH_3)_6$; it most certainly provides no palpable grounds for rejecting this picture.

(1) R. G. Vranka and E. L. Amma, *J. Amer. Chem. Soc.*, **89**, 312 (1967).
(2) H. C. Longuet-Higgins, *J. Chem. Soc.*, 139 (1946).
(3) S. K. Byram, J. K. Fawcett, S. C. Nyburg, and R. J. O'Brien, *Chem. Commun.*, 16 (1970).
(4) M. J. S. Dewar and D. B. Patterson, *ibid.*, 544 (1970).
(5) Note that III depicts these as being very unequal, which is a gross misrepresentation.

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