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Task No. NR 055-427

TECHNICAL REPORT NO. 15

Boron-11 Decoupling Studies on the Proton Nmr of $C_2B_4H_8$

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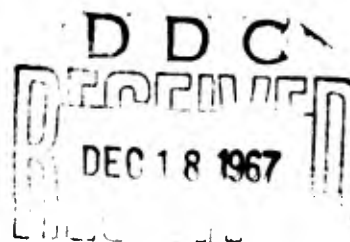
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December, 1967



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Boron-11 Decoupling Studies on the Proton Nmr of $C_2B_4H_8$

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The proton nmr of $C_2B_4H_8$ has been recorded and consists of a single peak $\tau = 3.68$, a 1:1:1:1 quartet $\tau = 6.56$, another 1:1:1:1 quartet $\tau = 10.13$, and a broad peak $\tau = 12.6$ which have been assigned to the H-C, $H_{\text{terminal-B}_{4,5,6}}$, $H_{\text{terminal-B}_1}$ and H_{bridge} hydrogen nuclei, respectively.¹ The assignment of the high field quartet to $H_{\text{t-B}_1}$, however, was based more on analogy² than on direct evidence. On this assumption it was necessary, from area considerations, to assign the low field quartet to two overlapping resonances, $H_{\text{t-B}_{4,6}}$ and the chemically unique $H_{\text{t-B}_5}$. Without direct evidence available there still remained the ambiguity of the $H_{\text{t-B}_1}$ and $H_{\text{t-B}_5}$ assignments. With this in mind the present study was undertaken.

The structure of $C_2B_4H_8$ has been verified by X-ray studies³ and it is clear that each of the basal boron atoms (4,6 and 5) of the pentagonal pyramidal framework has, in addition to a terminal hydrogen, an attached bridge hydrogen(s) whereas the apex boron has an attached terminal hydrogen only. With boron-11 decoupling experiments carried out at 19.2 Mc it is possible to selectively irradiate the high- and low-field proton nmr quartets. When the high field quartet is collapsed the rest of the spectrum remains unchanged. In striking contrast, collapse of the low field quartet is accompanied by a markedly sharpened bridge

hydrogen region. Such observations are consistent only with the original H_t-B_1 (no bridge hydrogens) assignment to the high field quartet.

This work was supported in part by a grant from the Office of Naval Research.

References

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