

High Resolution Proton Magnetic Resonance in Fluorobenzene

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Gutowsky et al. resolved the proton nuclear magnetic resonance spectrum of fluorobenzene into a doublet and interpreted that it would refer to the case where the fluorine was equally coupled through electrons with the ortho-, meta- and paraprotons¹⁾. Baker also presented the same conclusion²⁾. But this conclusion is a quite perplexing one to the chemists, and we continued the efforts to resolve the spectrum further and observed that the components of the doublet were different in the intensity from each other, consistent with the observation by Gutowsky et al.¹⁾, each having the structure as shown in Fig. 1.

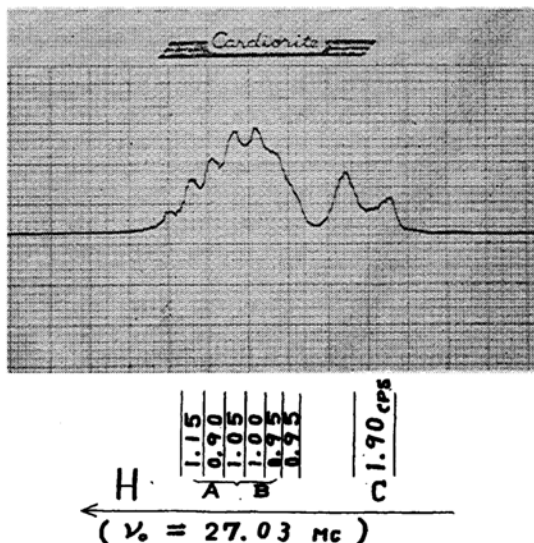


Fig. 1. Proton resonance in fluorobenzene.

The separation between each component of the multiplets is shown in Figure 1. In spite of the argument given by Baker²⁾ for the fluorine spectrum of this compound, we assume that the proton resonance spectrum of Fig. 1 would refer to the case where the effect of the non-equivalent distribution of electrons participates in

1) H. S. Gutowsky, L. H. Meyer and D. W. McCall, *J. Chem. Phys.*, **23**, 982 (1955).

2) E. B. Baker, *ibid.*, **13**, 984 (1955).

the resonance phenomena. A possible assignment of the line components may be done with the help of the molecular theory³⁾ by taking the peaks of A, B and C (A is the highest in the resonant field) as referring to meta-, para- and ortho-protons, respectively.

During this experiment, we could know that Bak, Shoolery and Williams⁴⁾ reached the same conclusion as ours of unequal H-F couplings, but, in their article, the spectrum of the proton resonance is not shown. Further efforts to make the assignments of each component line and to make measurements at higher field are now being on.

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3) For example C. A. Coulson: "Valence," Oxford University Press, (1953).

4) B. Bak, J. N. Shoolery and G. A. Williams, III, to be published in *J. Molecular Spectroscopy*.
