The NMR Spectrum of Acrylonitrile

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The NMR spectrum of acrylonitrile at the resonance frequency under 60 Mc. shows a very complicated ABC pattern, and the interpretation of the spectrum cannot be carried out without utilizing a high speed computer.

On the other hand, at the resonance frequency of 100 MC,* the spectrum showed a nearly AMX-type pattern (Fig. 1), and it was very easy to obtain the relative chemical shifts and spin coupling constants by using a simple rule of line splitting (case A).

A slightly more accurate treatment, in which the spin system was assumed to be ABX, was also carried out according to the method of Pople et al.[1] (caseB). In the latter case, the absolute values of each parameter were not

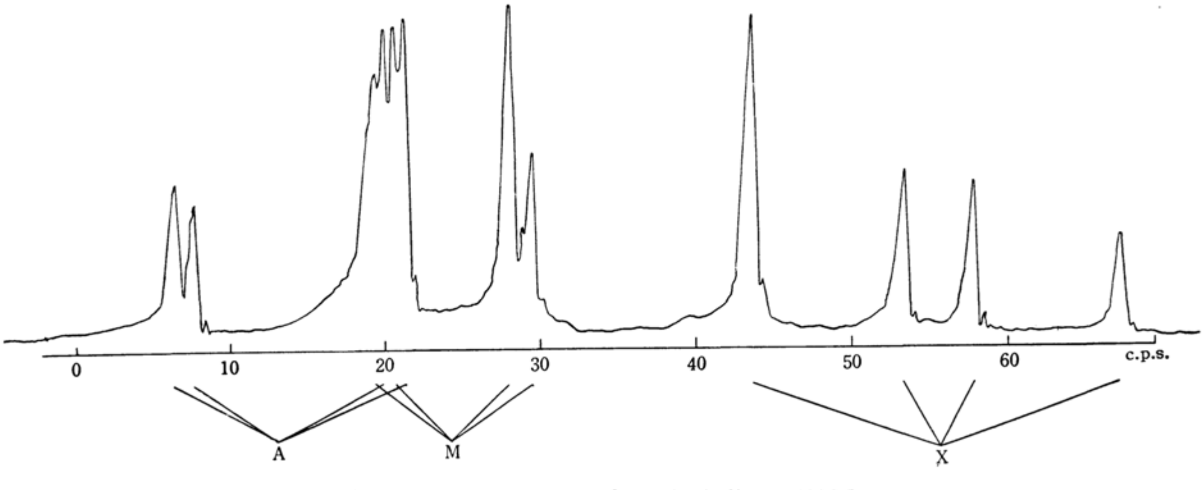

Fig. 1. NMR spectrum of acrylonitrile at 100 Mc.

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* The NMR spectrum was recorded with a Varian HR-100 spectrometer.

[1] J. A. Pople, W. G. Schneider and H. J. Bernstein, " High Resolution Nuclear Magnetic Resonance, " McGraw-Hill, New York (1959), Chap. 6.

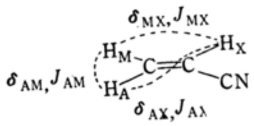

Fig. 2. Parameters for acrylonitrile.

TABLE I. CHEMICAL SHIFTS δ AND COUPLING CONSTANTS J OF ACRYLONITRILE (c. p. s.)

	δ_{AM}	δ_{AX}	δ_{MX}	J_{AM}	J_{AX}	J_{MX}
Case A	11.7	45.0	33.3	1.4	14.7	10.0
Case B	11.6	45.0	33.4	1.4	14.4	9.5
Castellano's Data[2]	10.0	47.9	37.9	1.7	18.0	11.0

essentially different from those of the former case. The relative sign between J_{AX} and J_{MX} (see Fig. 2), could, however, be determined to be positive in case B.

The results are illustrated in Table I, which compares them with the data obtained at 40 Mc. by Castellano et al.,[2] which data are reduced to the values at 100 Mc. The coincidence among these data is satisfactory.

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[2] S. Castellano and J. S. Waugh, *J. Chem. Phys.*, **43**, 295 (1961).