NMR Study of 3,5-Dichloropyridine in the Nematic Phase of the Liquid Crystal

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The importance of NMR studies on oriented molecules dissolved in the nematic phase of liquid crystals is well recognized [1]. The aim of this note is to report such a study of 3,5-dichloropyridine in the nematic phase of N-(p-Methoxy-benzyliden)-p-n-butylanilin (MBBA). The observed spectrum is that of an AB_2 symmetry with nine detected lines (Fig. 1). The analysis [1] of this spectrum is straightforward and the values for the direct (D) coupling constants, the indirect (J) coupling constants and the elements of the orientation matrix S are:

$$D_{AB} = -\ 51\ \text{Hz}, \qquad S_{11} = 0.003,$$
$$D_{BB} = -241\ \text{Hz}, \qquad S_{22} = 0.139.$$
$$J_{AB} = \pm\ 2\ \text{Hz},$$

J was supposed to have the same value as in the isotropic phase and elements of the S matrix were obtained by using the geometry of pyridine [2]. The values of D suggest that the molecule is preferentially oriented with the axes B–B along the magnetic field. The anisotropies of the chemical shifts are $\sigma_a = 0.46$ ppm for protons A and $\sigma_a = 0.06$ ppm for protons B. These shifts are towards higher fields and support the mentioned conclusion about the orientation of the molecule. We could not explain in a simple manner why the chemical shifts are so different for A and B protons.

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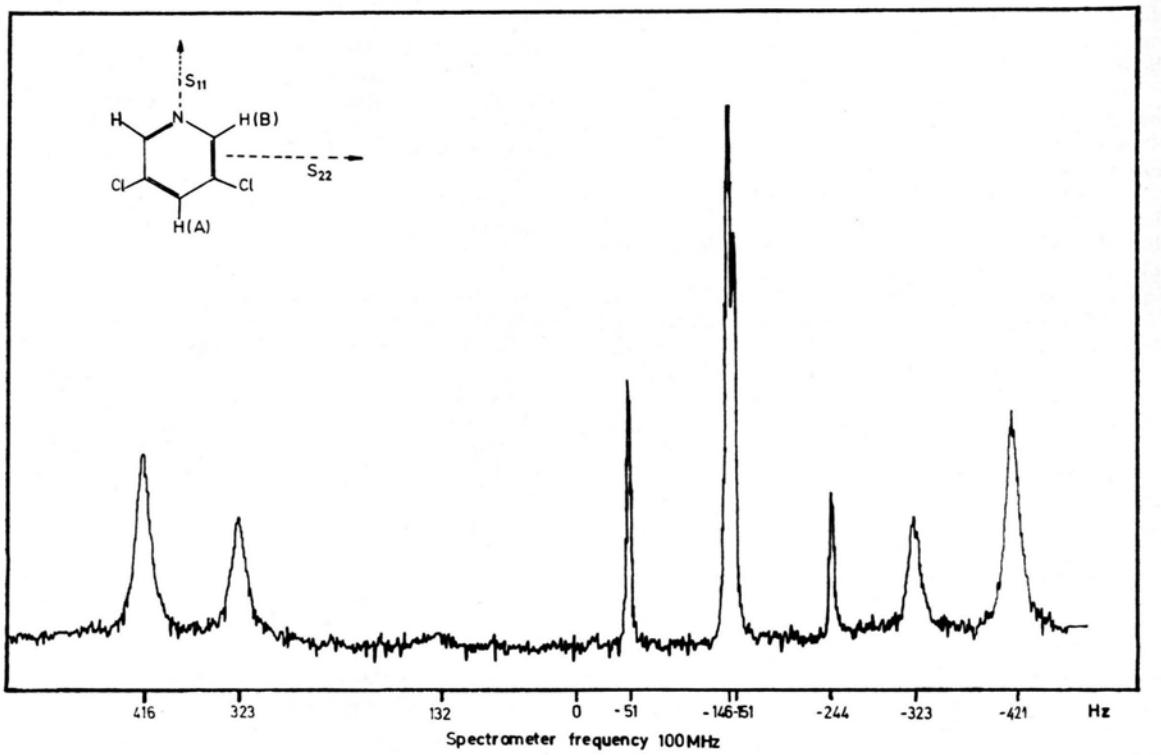

Fig. 1. The spectrum of an AB_2 symmetry with nine detected lines.

[1] P. DIEHL and C. L. KHETRAPAL, NMR Basic Principles and Progress, Vol. 1, ed. P. DIEHL, E. FLUCK, and R. KOSFELD, Springer-Verlag, Berlin 1969.

[2] Tables of Interatomic Distances and Configuration in Molecules and Ions, ed. L. E. SUTTON, Special Publication No. 18, Chemical Society, London.