NMR Spectra of $CH_3(D_3)COOH$ and CF_3COOH in Nematic Liquid Crystals

D. Pumpernik and A. Ažman

Chemical Institute Boris Kidrič, University of Ljubljana, Ljubljana, Yugoslavia

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NMR spectra of oriented $CH_3(D_3)COOH$, CF_3COOH in various liquid crystals are given. The quadrupole coupling constant of CD_3COOH is evaluated.

In this note we report H, F and D spectra of $CH_3(D_3)COOH$ and CF_3COOH in various liquid crystals. The results (Table 1) include: the direct coupling constants (D), splitting of the doublet in the deuterium spectra (Δ), the z components of the S matrix and the calculated quadrupole coupling constants. Due to the $(-O-H)$ proton exchange there is no coupling between this proton and the CH_3 or CF_3 group. The symmetry of all these systems is therefore C_3. The direct coupling constants for the F atom in CF_3COOH are the same in Merck V and in MBBA (N-(p-Methoxy-benzyliden)-p-n-butylanil). For CH_3COOH the values of D are roughly the same in Merck V, IV and HOAB (4-4′-di-n-heptyloxyazoxy benzene) but differ considerably from the value in MBBA. The calculated quadrupole coupling constants [1] (the geometries of the compounds from Ref. [2]) have almost the same value. Therefore there is no specific interaction of CH_3COOH with the liquid crystals and the large differences of D reflect the influence of the dissolved species on the liquid crystals orderings. The addition of CF_3COOH to Merck V and of MBBA or CH_3COOH to MBBA, disturbes the ordering of the liquid crystals to a much greater extent than the addition of CH_3COOH to Merck V, IV or HOAB. The calculated value of the quadrupole coupling constant of CD_3COOH falls in the range of quadrupole coupling constants observed so far [1].

The spectra were recorded with a JEOL PS-100 instrument. The temperatures of the system were 18° for Merck and MBBA liquid crystals and 94° for HOAB.

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System	Liquid crystal	D (Hz)	Δ (kHz)	S_{zz}	e^2qQ/h (kHz)
CF_3COOH	Merck V	271		$1.23 \cdot 10^{-2}$	
	MBBA	270		$1.22 \cdot 10^{-2}$	
CH_3COOH	Merck V	1550	11.4	$1.38 \cdot 10^{-1}$	178
	Merck IV	1850		$1.64 \cdot 10^{-1}$	
	HOAB	1550		$1.38 \cdot 10^{-1}$	
	MBBA	190	1.5	$1.69 \cdot 10^{-2}$	185

Table 1. Direct coupling constants D, splittings in the deuterium spectra Δ, z components of the S matrix, and quadrupole coupling constants e^2qQ/h.

Reprint requests to Dr. A. Ažman, Dept. of Chemistry University of Ljubljana, Murnikova 6 — P.O.B. 537, *J-61001 Ljubljana*, Jugoslawien.

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BERICHTIGUNG

Zu H. Schirmer und I. Stober, „Zur näherungsweisen Berechnung der elektrischen Leitfähigkeit eines Plasmas", Zeitschrift für Naturforschung **28 a**, 1454–1458 [1973]. Auf Seite 1457 sind die Abb. 2 und 3 vertauscht.