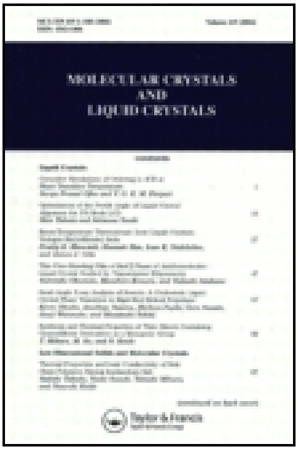

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UNIAXIAL ROTATION BIASING IN Sm E LIQUID CRYSTALS

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Abstract The polar and bipolar uniaxial molecular rotational biasing effect as described by the model of the on an circular arc confined simple rotational diffusion, have been investigated on the Sm E phase neutron incoherent elastic structure factor, as well as on the asymmetry parameter of the electric field gradient tensor.

INTRODUCTION

The model of the uniaxial, on the segment of the circle of an apex angle Φ_0, restricted rotational diffusion of the proton explains the MBBA nematic phase incoherent neutron scattering data[1], as well as the published[2] temperature dependence of the deuteron spin-lattice relaxation of $5CB\text{-}d_{15}$ nematic compound.

In general, the evidence that the uniaxial molecular rotation is in Sm phases restricted, is provided for by the incoherent neutron scattering[3], or by ^{14}N NQR measurements[4] of the asymmetry parameter, η.

THEORETICAL OUTLINE

The orthogonal two-dimensional lattice of the Sm E phase is characterized by the herringbone molecular arrangement of the long range, fig.1. In order to investigate *directly* the possible polar *or* bipolar uniaxial molecular rotation biasing effect *in Sm* E phase, we assign the in-plane

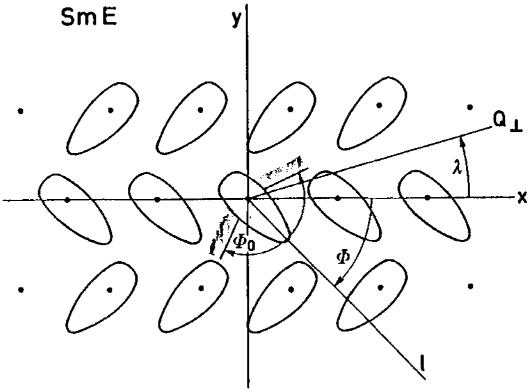

FIGURE 1 Herringbone arrangement of the Sm E phase molecular in plane structure showing the angular separation of the potential barriers restricting the molecular uniaxial rotation.

orientational order of each particular molecule to the average orientation of its transverse molecular axis, which in terms of the model of the biased uniaxial molecular reorientation described above is represented by the bisector of the circular segment, fig. 1.

Characteristic feature of this model is the fact, that the expressions related to the restricted proton stochastic reorientations (with respect to the segment bisector, denoted by l in fig. 1) is given by,

$$< e^{ik\gamma} > = j_0\left(\frac{k\Phi_0}{2}\right), \tag{1}$$

where j_0 is the spherical Bessel function of the order 0, and γ is the Euler angle denoting the instantaneous proton position with respect to the line of nodes. The reorientation of the molecule takes place around its long axis, which on the average coincides with the z – axis of the laboratory system, fig 1. The orientation of the segment bisector with respect to the laboratory frame (i.e. the line of nodes l) is described by Euler angle ϕ. In fig. 1, $Q_\perp$ denotes the projection of the neutron scattering vector Q onto the smectic E plane.

The elastic incoherent structure factor, EISF, to be evaluated reads[3], $A_0 = |< e^{iQR} >|^2$, where R denotes the position vector of the proton. EISF, which describes the *geometry* of the localized proton motion[3] has been derived for two orientations of Q. The results (averaged over the angle λ) are the following:

$$A_{0\parallel} = \left[J_0(Qa\sin\Theta) + 2\sum_{k=1}^{\infty} J_{2k}(Qa\sin\Theta)\, j_0(k\Phi_0)\right]^2, \qquad (2)$$

$$A_{0\perp} = \sum_{k=1}^{\infty} s_k s_k^{*}\; j_0^2\left(\frac{k\Phi_0}{2}\right) J_k^2\left[Qa\cos^2\left(\frac{\Theta}{2}\right)\right], \qquad (3)$$

where Θ denotes the angle between the z'-body frame and z-laboratory axis system, a is the radius of the circle, and the in-plane order parameter is defined as $s_k = < e^{ik\phi} >$, where ϕ is the angle between l and the laboratory x-axis. The simbols $\parallel$ and $\perp$ describe the parallel and perpendicular orientation of a vector Q with respect to the director n_0. J_k denotes the k-th order cylindrical Bessel function. The eq. (3) is an approximation valid for $\Theta < 60^{o}$, say.

The averages over ϕ have been evaluated for the two model in plane distribution functions, describing the preferential orientation of the outboard transverse molecular axes: (a) $P(\phi) = \phi\, e^{-\phi}/\Gamma(2.4)$, and (b) $P(\phi) = \cos^2(\phi - \xi)/\pi$ describing the polar (a), and the bipolar, (b), distributions. An example of the results is presented in fig. 2. It turns out that the spread of calculated EISF curves, as a function of the parameter Φ_0, are very sensitive to the choice of the distribution functions, the exact form of which is unknown.

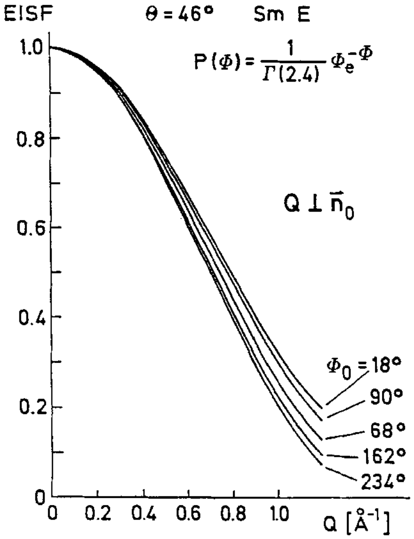

FIGURE 2 The EISF curves calculated in perpendicular orientation of Q for the polar in plane distribution.

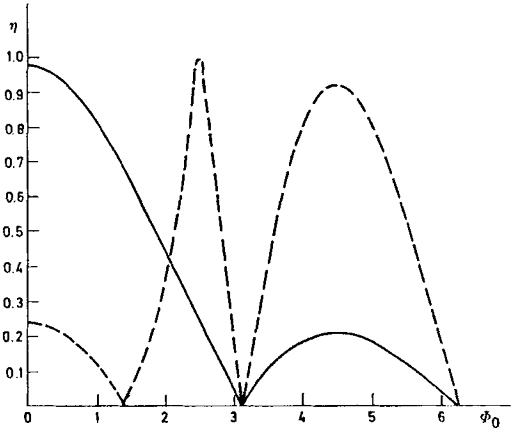

FIGURE 3 The asymmetry parameter, η, calculated for the bipolar Sm E biased rotation.

For the above model of the restricted reorientation, the ^{14}N NQR asymmetry parameter reads (taking Θ = 0 in Sm E phase):

$$\eta = (2/V_{33})\left[V_{12}^2 + \frac{1}{4}(V_{11} - V_{22})^2\right]^{1/2} j_0(\Phi_0)\langle\cos 2\phi\rangle$$

for the bipolar, and

$$\eta = \frac{2(V_{13}^2 + V_{23}^2)}{3 V_{33}^2} \; j_0^2\left[\frac{\Phi_0}{2}\right] \langle\cos\phi\rangle^2$$

for the polar ordering. Here, V_{ij}, represents the ij-th

^{14}N EFG tensor element in the molecular frame in the solid state[4]. Taking the limit $\Phi_0 \rightarrow 0$, the exact formal expressions of ref.[4] for Sm IV phase are obtained. If we, however, now interprete the $\langle \quad \rangle$ term as being associated with the structural property of the phase and is therefore constant, then the whole temperature dependence is presumably hidden in the variation of the angular separation, Φ_0, between the two potential bariers available to the proton (or to the ^{14}N nucleus). The Φ_0 dependence of η, as shown in fig. 3 for the bipolar case,(full line $\langle\cos 2\phi\rangle=0.23$ and dotted line $\langle\cos 2\phi\rangle=1.00$) do indeed exibit the major characteristic features (monotonic decrease or increase but also in the Sm C observed maximum) reported in ref.[4], are now, in terms of the proposed model above, immediately amenable to simple physical interpretation.

CONCLUSIONS

It is suggested, that the model of uniaxial restricted stochastic reorientation allows the detailed investigation of a polar or bipolar type of biased molecular rotational motion occuring in smectic liquid crystals.

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