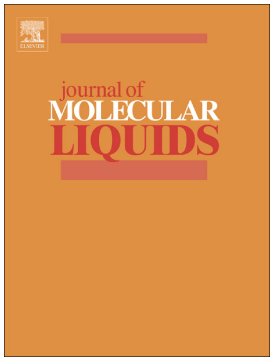

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Molecular dynamics of 4-propyl-4′-thiocyanatobiphenyl (3BT) in the strong glass-forming smectic E phase

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ABSTRACT

Broadband dielectric spectroscopy was employed to study glass transition dynamics in highly ordered smectic E phase of 4-propyl-4'-thiocyanato-1,1'-biphenyl (3BT). Three relaxation processes exhibiting Arrhenius-like thermal activation were detected: (1) δ-relaxation assigned to molecular reorientation around the short axis, (2) α-relaxation attributed to rigid molecular cores tumbling around the long axis and (3) secondary β-relaxation. Our investigations revealed that the smectic E phase (SmE) is a *strong* glass-former with the smallest possible fragility index m_f~16. Finally, an analysis of loss spectra ($\varepsilon''(f)$) in terms of their shape parameters (1-*m*) and *n* demonstrated long and short range coupling between molecular motions in the glassy state.

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1. Introduction

In general, glass is defined as a solid material in a metastable state lacking any long-range positional and orientational molecular arrangement. However, glasslike behaviour has also been observed in so called plastic crystals, which are characterized by a random orientation of molecules forming a crystal lattice. Generally, glass-forming materials can be classified as *strong* or *fragile* with respect to their relaxation pattern [1]. *Strong* glass-formers typically show Arrhenius relaxation processes, while the temperature dependence of relaxation rates in *fragile* glass formers is described by the empirical Vogel–Fulcher–Tamman (VFT) equation given as

$$\tau_\alpha(T) = \tau_\infty \exp\left(\frac{E_v}{R(T-T_v)}\right), \qquad (1)$$

where τ_∞ is the so-called pre-exponential factor, and E_v and T_v are the 'Vogel activation energy' and the Vogel temperature, respectively. A measure of the response of glass forming systems to temperature changes is the so-called fragility index, defined by the slope at T_g in the plot of $\log_{10}(\tau_\alpha)$ versus T_g/T:

$$m_f = \left.\frac{d\log(\tau)}{d(T_g/T)}\right|_{T=T_g}, \qquad (2)$$

Strong glass-formers are characterised by an m_f value of ~16, and the most fragile systems by a value as high as 200. Combined structural and viscosity investigations suggest the presence