

QENS Studies of Fast Molecular Reorientations in Isotropic, Cholesteric, Glass and Crystalline Phases of 5*CB

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Chain branching and chirality of molecules affect various physical properties substantially, such as the phase behavior. We have been interested in phase relation and dynamics of some chiral molecules that form a liquid crystalline phase. Here, we report the results obtained from neutron scattering experiments for isopentyl cyanobiphenyl (5*CB).

5*CB has a cholesteric phase, whereas 5CB, which is an enantiomer of 5*CB, has a nematic phase. The calorimetric measurements as well as the dielectric relaxation measurements have already been made [1]-[4]. The isotropic liquid is easily under-cooled to form a cholesteric phase, which is metastable and forms a glass on further cooling below 210 K. There exist two crystalline phases (metastable and stable). The dielectric relaxation measurements showed that the molecular reorientational motion along the short axis becomes quite slow near the glass transition temperature of 210 K. The purpose of this experiment was to investigate the molecular reorientational motion along the long axis and the internal molecular motions.

We performed neutron scattering experiments on 5*CB using the AGNES spectrometer at JRR-3M. The measurements were made at 350 K, 325 K, 300K, 275 K, and 250 K for the isotropic liquid and at 225 K for the cholesteric phase with a low-resolution mode ($\Delta E = 120$ micro-eV), and also at 350 K and 300 K with a high-resolution mode ($\Delta E = 49$ micro-eV). As a reference sample, 5CB was also investigated at 350 K and 325 K for the isotropic-liquid and at 300 K for the nematic phase with a low-resolution mode.

First, we assumed that the spectra obtained were convoluted with a delta func-

tion (an elastic component) and a Lorentz function (a quasielastic component). However, the fitting was not quite. Next, we tried to fit the data with two Lorentz functions, which was actually better. So, we might have observed the diffusional motion as well as the reorientational motion. The high-resolution spectra were also fitted well with two Lorentz functions, and the HWHM was similar to that obtained from the low-resolution spectra. The narrower component can be assigned to the translational diffusion of the molecule and the wider component to the reorientational motion, presumably the reorientational motion around its long axis. The HWHM of the narrow component is plotted against the momentum transfer (Q) to determine the diffusion constant at each temperature. An Arrhenius plot for the diffusion constants gives an activation energy of 15.1 kJ/mol (Fig. 1), indicating that the diffusion constant does not affected by the isotropic-cholesteric phase transition. For the wide component, there still remains the possibility that there is complicated reorientational motions.

The 5CB spectra could also be fitted by two Lorentz functions. The HWHM of the narrow component was significantly broader than that for 5C*B, indicating that the diffusive motion of 5*CB is slower than that of 5CB. The activation energies obtained are very similar for both compounds.

It is also interesting to know the difference in the vibrational DOS among three phases of 5*CB, the glassy cholesteric phase, metastable crystal and the stable crystal. The heat capacity of the metastable crystal at low temperature (below 70 K) was significantly smaller than that of the

stable crystal, while the metastable crystal has glass transition at 100 K. The inelastic incoherent neutron scattering revealed that the stable crystal had larger DOS than the metastable crystal at low energies around 1.5 meV, which is consistent to the result obtained by calorimetry [4].

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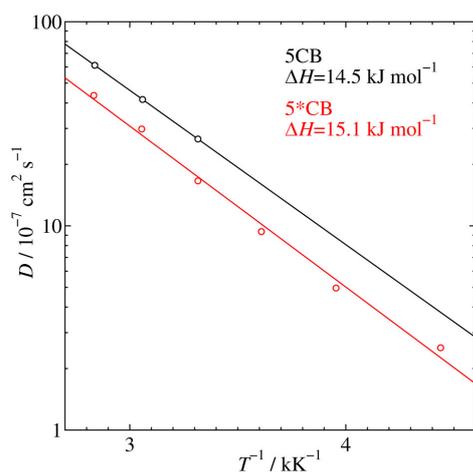


Fig. 1. An Arrhenius plot of the diffusion constant obtained for 5*CB and 5CB