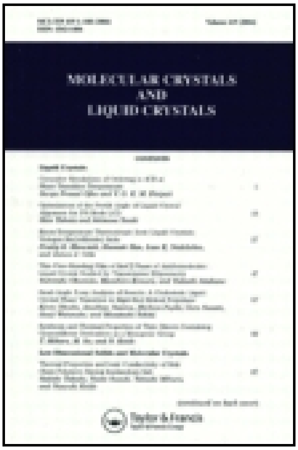

Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals

Orientational Behavior of Discotic Nematic Phase for a Discotic Liquid Crystalline Triphenylene on Polyimide and Alkylammoniumbromide Coated Substrates

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Orientational Behavior of Discotic Nematic Phase for a Discotic Liquid Crystalline Triphenylene on Polyimide and Alkylammoniumbromide Coated Substrates

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Orientational behavior of a discotic liquid crystalline triphenylene (C8OBT) on the substrates coated with a polyimide and a cetyltrimethylammoniumbromide (CTAB) was investigated by polarizing microscopy. The averaged direction and the order parameters of the triphenylene core plane and carbonyl groups of C8OBT were evaluated by an infrared dichroic method. C8OBT exhibits a homeotropic alignment on a polyimide film as for the discotic nematic (N_D) phase, while it shows a tilt or homogeneous alignment on a CTAB-coated substrate. The order parameter of triphenylene N_D phase is higher on the polyimide ($S = 0.6$) than a CTAB-coated substrate (0.2), in contrast to that of the carbonyl groups is comparable (0.2).

Keywords discotic liquid crystal; alignment; discotic nematic phase; order parameter, triphenylene

INTRODUCTION

One of characteristic features of liquid crystals, especially for nematic liquid crystals is the better controllability of molecular alignment by the surface effect. At present, a rubbed polyimide-coated substrate is widely used to obtain a homogeneous alignment of rod-like liquid crystals.[1] An optical compensation film for TFT-LCDs was a most successful application of discotic liquid crystals, while ND phase was utilized to obtain an objective alignment of mesogene by polymerization. The molecular alignment behavior and controllability are quite essential and significant in device fabrications as an application. Therefore, it is essentially important to understand the mechanism of molecular alignment at the interface between discotic liquid crystals and substrates.

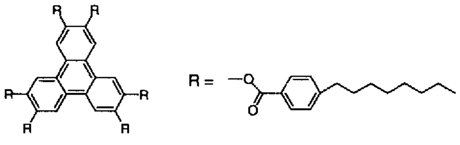
However, there are only several reports about the orientational behavior of discotic liquid crystals[2-6] in comparison with those of rod-like systems. Several studies have been reported for the molecular alignment and the order parameters in the uniformly aligned columnar phase of discotic liquid crystals measured by an infrared dichroism. Kruk *et al.* have reported the order parameter of a columnar discotic liquid crystal.[2] According to this method, the order parameter was evaluated by using unpolarized infrared radiation and comparing the IR absorption intensity for the columnar phase with that of the isotropic phase. This method is useful for analyzing molecular alignment mechanism of liquid crystals because of the ability to evaluate the averaged direction of functional groups in the molecule by the order parameters. On the other hand, Favre-Nicolin *et al.* reported the order parameters in ND phase of acrylate derivatives of triphenylene calculated from the refractive index using the Vuks approximation.[6] However, those were for the alignment of the whole molecules in a scope of optical property. The dependence of the alignment and the order parameter for each functional groups in N_D phase on the substrates coated with an organic layer have not yet been studied in detail.

In this work, orientational behavior of 2,3,6,7,10,11-hexa(4-*n*-octyloxybenzoyloxy)triphenylene (C8OBT) on a spin-coated polyimide (JSR Co. Ltd., AL1254) film and a cetyltrimethylammoniumbromide (CTAB) coated substrate was investigated by a polarizing microscope with a hot stage and the order parameters were evaluated by FT-IR spectroscopy.

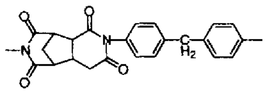
EXPERIMENTAL

C8OBT shows three enantiotropic phase transitions.[5,7] The two mesophases, the rectangular columnar (Col_r) and N_D phases appears (C 150 Col_r 167 N_D 238 Iso). A polyimide film was prepared by spin-coating technique at 3000 rpm for 3 minutes on a well-cleaned glass substrate. Then it was heated at 90 °C for 1 minute, followed by drying at 180 °C for 1 hour. This film was not treated by rubbing. The thickness of the obtained polyimide film was estimated to be *ca.* 45 nm by ellipsometry. A CTAB-coated substrate was prepared by dipping glass plates in a saturated aqueous solution of CTAB. C8OBT was sandwiched between these substrates with silica beads (2-μm diameter) spacer. For infrared spectra measurements, BaF_2 plates were used instead of glass plates. The textures of N_D phase were observed by a polarizing microscope with a hot stage. The temperature dependence of FT-IR spectra was measured in order to evaluate the directions and the order parameters for the triphenylene core and the carbonyl groups of

C8OBT. The order parameters were evaluated by infrared dichroism following the method of Kruk *et al.*[2] and the averaged direction is estimated from the dichroic ratio between the isotropic phase and mesophase.



C8OBT



AL1254

CTAB

RESULTS AND DISCUSSIONS

As shown in Figures 1(a) and (b), C8OBT showed a typical nematic schlieren texture on a glass substrate, while a homeotropic texture was observed on the polyimide film in N_D phase. On the other hand, the texture on a CTAB-coated substrate showed a tilt or homogeneous texture that optical axes of molecules aligned sideward or parallel to the substrate (Figures 1(c) and (d)). The results indicate that the molecular plane is uniformly parallel to the substrate on the polyimide, while that on the CTAB has a tendency to align perpendicular to the substrate.

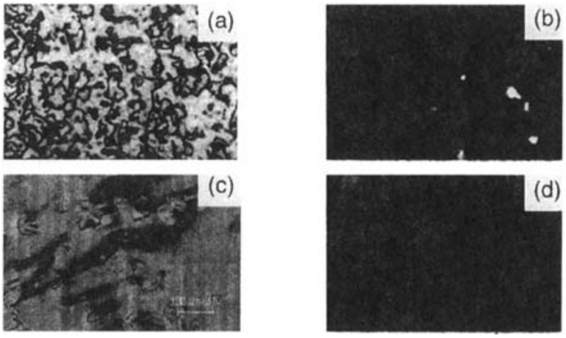


FIGURE 1 Textures of N_D phase (200 °C) for C8OBT, cooled from the isotropic phase sandwiched by glass plates with (a) non-coating, (b) polyimide films, (c) CTAB, and (d) after the sample was rotated by 45° around the optical axis from (c).

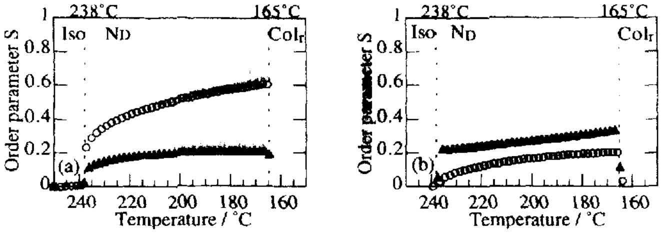


FIGURE 2 Temperature dependence of the order parameters for the C=O str. at 1745 cm^{-1} (▲) and the aromatic C=C str. at 1603 cm^{-1} (○). (a) on a polyimide film and (b) on a CTAB one.

The temperature dependence of the order parameters of the triphenylene core and the carbonyl groups were evaluated as shown in Figure 2.[8] The order parameter of the triphenylene core on the polyimide (S = 0.6) was higher than that on the CTAB-coated substrate (0.2), though the carbonyl groups showed a comparable value (0.2) in N_D phase. The results agree with the results of the polarizing microscopic texture observation in N_D phase. We believe that the triphenylene core of C8OBT was strongly anchored parallel to the polyimide, while it loosely aligns vertically to the CTAB substrate. The quantitative evaluation of the alignment of each groups will be applicable for understanding the mechanism of molecular alignment at the interface between discotic liquid crystal and substrates.

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[8] The relative IR absorption intensity R can be defined by $R = I_{N_D} / I_{Iso}$, where the I_{N_D} is the integrated absorbance of the band in the N_D phase and I_{Iso} is that in the isotropic phase. Using the calculations by Neff *et al.* for unpolarized radiation I_{N_D} is defined by $I_{N_D} = \cos^2\alpha <\sin^2\theta> + \sin^2\alpha <1 + \cos^2\theta>$, where α is the angle between the functional group and the normal to the substrate, and θ is the angle between the direction of the transition dipole moment and the direction of an incident IR light. The order parameter S is defined by $S = 2(R - 1)$ (at $\alpha = 90°$) and $S = 1 - R$ (at $\alpha = 0°$).