Experimental Report

Proposal: **6-05-930** **Council:** 10/2012

Title: Elastic Sans on a Homologous Series of Discotic Liquid Crystals

This proposal is a new proposal

Researh Area: Soft condensed matter

Main proposer: **SCHOENHALS Andreas**

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Local Contact: FRICK Bernhard

Samples: 2,3,6,7,10,11-hexa-[n-alkonoyloxy] triphenylene (HOTn; n=6,8,10,12)

Instrument	Req. Days	All. Days	From	To
IN16	3	3	13/05/2013	16/05/2013

Abstract:

Discotic liquid crystals (DLC) are soft-matter materials which organize into columns that further assemble into two-dimensional arrays with a hexagonal mesophase. Highly ordered columnar structures were found to be very promising as active semiconductors in organic field-effect transistors and photovoltaic devices. The charge transport in these systems is controlled by their molecular mobility. To get an overview about the molecular mobility in DLCs at a time scale of ca. 2 ns it is proposed to carry out elastic scans on a backscattering instrument on the homologous series of DLCs 2,3,6,7,10,11-hexa-[n-alkonoyloxy] triphenylene (HOTn; n=6,8,10,12) in the bulk state.

EXPERIMENTAL REPORT

EXPERIMENT N°6-05-930 INSTRUMENT IN16

DATES OF EXPERIMENT 13/05/2013-16/05/2013

TITLE

Elastic Sans on a Homologous Series of Discotic Liquid Crystals

EXPERIMENTAL TEAM

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Discotic liquid crystals (DLC) are self-assembled materials where self-assembly is driven by noncovalent intermolecular interactions [1]. DLCs consist of a flat and rigid aromatic core substituted by flexible aliphatic side chains. The former is responsible for the π-stacking and the latter for the increased solubility, processability, and rich thermotropic behavior. The disc-shaped molecules organize into columns that further assemble into two-dimensional arrays with a hexagonal mesophase. The alkyl chains fill the intercolumnar space giving rise to a nanophase separated state.

To have an overview about the microscopic dynamics elastic scans are carried out at IN16 on a homologous series of discotic liquid crystals based on 2,3,6,7,10,11-hexa-[n-alkonoyloxy] triphenylene (HOTn; n=6,8,10,12) in the bulk state. The experiments were done on IN16 (λ=6.271 Å; 'unpolished' Si-111). All measurements were corrected for the scattering of the empty can. Assuming a Gaussian form for the elastically scattered intensities the effective mean square displacement $\langle r^2 \rangle_{eff}$ is extracted in its temperature dependence.

As an example Figure 1 gives the the effective mean square displacement $\langle r^2 \rangle_{eff}$ for HOT6. Besides the phase transitions of HOT6 visible as steps in the temperature dependence of the scattered intensity, different regimes of molecular mobility can be identified. Around T=150 K the rotations of the methyl groups can be observed as a small step in $\langle r^2 \rangle_{eff}$ versus temperature followed by a step at around 300 K which resembles features of a thermal glass transition. This will be investigated in further detail.

Figure 2 gives the mean squared displacement $\langle r^2 \rangle_{eff}$ in the columnar liquid crystalline phase versus the core-core distance of the columns estimated by X-ray difraction. As expected the $\langle r^2 \rangle_{eff}$ increases with increasing n and therefore with increasing core-core distance between the columns. For the corresponding series of the HATn materials a corresponding dependence is obtained for smaller n.

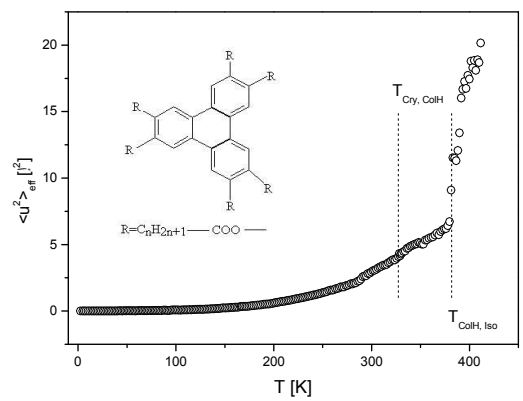

Fig. 1: Effective mean squared displacement $\langle r^2 \rangle_{eff}$ versus temperature for HOT6. The inset gives the chemical structure of 2,3,6,7,10,11-hexa-[n-alkonoyloxy] triphenylene. Dashed lines give the phase transitions for HOT6.

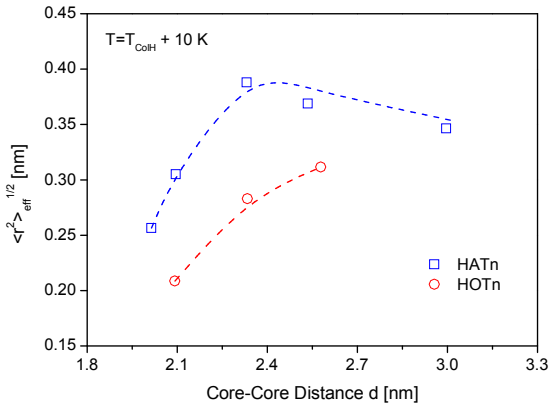

Fig. 2: Effective mean squared displacement $\langle r^2 \rangle_{eff}$ versus the core-core distance: Squares –HATn; Circles – HOTn. Dashed lines are guides for the eyes.