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# Molecular Crystals and Liquid Crystals

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# New Liquid Crystalline Structures in the Series Of 2-(Trans; 4-N-Alkylcycloheayl)-Propan-1, 3-Diols

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NEW LIQUID CRYSTALLINE STRUCTURES IN THE SERIES OF 2-(TRANS 4-n-ALKYLCYCLOHEXYL)-PROPAN-1,3-DIOLS

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# INTRODUCTION

Specific interactions of parts of molecules have led to new structural models in the field of liquid crystals. The polar cyano group, may for example cause a "bi-layered" or "partially bi-layered" structure of the smectic A type. Hydrogen bridges in carboxylic acids yield dimers which produce a "bi-layered" structure in the smectic C phase 1. A variation of this concept seems to be realized in 2-(trans 4-n-alkylcyclohexyl)-propan-1,3-diols.

#### RESULTS

The compounds were prepared as intermediates in the synthesis of derivatives of 5-cyclo hexyl-1,3-dioxan <sup>2</sup>. The synthesis was performed according to figure 1, where trans-isomers are involved.

The trans-isomers were separated by recrystallization from hexane.

#### FIGURE 1

In the following we refer to the hexyl homologue of the diol, only.

The preliminary microscopic investigations with polarized light led to the following transition scheme

$$Cr = S_B = \frac{110^{\circ}C}{S_A} = S_A = \frac{114.5^{\circ}C}{S_A}$$
 is

Detailed texture and miscibility investigations will be reported in a separate paper <sup>3</sup>.

The unaxial character of the phases was proved by conoscopic investigations.

The X-ray studies were performed using Guinier equipment as well as a flat-film method in connection with oriented samples.

Figure 2 displays the pattern of the  $\mathbf{S}_{\mathtt{A}}$  phase. The molecules are oriented perpendicular to the magnetic field and perpendicular to the smectic layers (The direction of the magnetic field is marked by an arrow).

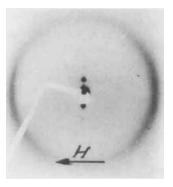


FIGURE 2

The diffuse scattering at Bragg-angles of about  $10^{\circ}$  is a characteristic feature of the  $S_A$  phase. As a special feature, a remarkably high number of orders of the layer reflection (up to the 4 th order) can be observed. The corresponding d-value is 27.5 %. In comparison with the molecular length a ratio d/L = 1.6 is obtained.

The position of the inner ring does not show any alteration at the transition into the low temperature phase.

The Guinier pattern of this phase shows three outer reflections (figure 3), which were indexed on the basis of a hexagonal lattice ( $a_{\rm hex}$ =5.93Å). Up to now, a similar pattern has not been observed in  $S_{\rm B}$  phases. It proves the high structural order in the phase under discussion.

Further investigations are necessary to clarify the situation.

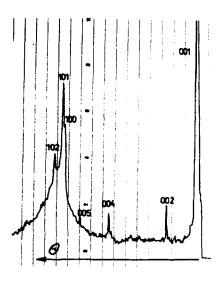


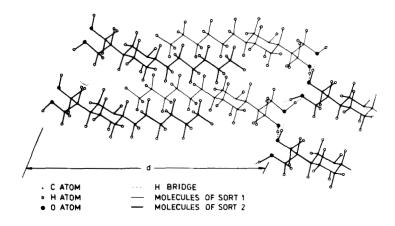
FIGURE 3

The d-value of 27.5 Å is explained by a model given in figure 4.

The evidence for the model is obtained from investigations of further homologues which will be reported later  $^3$ .

The sketched hydrogen-bridges were indicated by spectroscopic measurements. According to these measurements free O-H bands were not detected.<sup>4</sup>

In figure 4 the molecules of sort 1 and sort 2 are shifted with respect to each other in the direction of view. However, the assumed model must be proved by an exact structure analysis.



## FIGURE 4

It should be mentioned that similar structures (with respect to the interdigitation of the alkyl chains) have been reported for derivatives of glycopyranosides in the crystalline state  $^{5, \ 6}$ .

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