22.1-06 X-RAY DIFFRACTION BY 4 - ACETYL - 4' - *n* - ALKANOYLOXY - AZOBENZENES LIQUID CRYSTALS.

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The preparation and melting behaviour of the homologous series of 4 - acetyl - 4 - *n* - alkanoyloxy - azobenzenes $CH_3 - CO - C_6H_4 - N = N - C_6H_4 - O - CO-(CH_2)_n - CH_3$

(with *n* ranging from zero to 16) was recently reported (G. Poeti, E. Fanelli, M. Braghetti, Mol. Cryst. Liq. Cryst. 45 (1978) 145). This series was investigated by X-ray diffraction. In particular the disordered mesophases, namely the nematic and smectic phase, were considered. The dependence of the smectic A interlayer distance as a function of '*n*' appears to be of particular interest.

22.1-07 CRYSTALLOGRAPHIC AND CONFORMATIONAL STUDY OF DISK-LIKE HEXAESTERS (AND ETHERS) OF TRIPHENYLENE.

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Hexaesters and hexaethers of triphenylene (T) are known to give one or several mesophases for some length of their alkyl chains. Such mesophases belong to the exotic, newly discovered family of discotic liquid crystals.

Three hexaesters with propyl, butyl and pentyl chains have been crystallized and their structure investigated (Up to now no crystalline structure of disk-like compound has been yet published).

The six COOCn H_{2n+1} ester chains of each molecule are approximately perpendicular to the T core, and alternatively directed above and under its plane. Molecules are associated in pairs, with their T cores parallel and 3.43 Å away, and arranged in a hexagonal lattice ($R\bar{3}c$ space group) for the propyl ester. For the butyl- and pentyl esters the lattice is slightly distorted and becomes monoclinic (C2/c space group) with pseudohexagonal symmetry. However the molecules are arranged in a very similar manner for the three compounds.

Semi-empirical calculations have been performed in order to simulate the discotic mesophasis; preferential molecular conformations for the isolated molecule, association of molecules in pairs, and possible arrangement of dimers in columns have been computed for different lengths of alkyl chains.

The molecular geometry of dimers is independent of the chain length. On the other hand a drastic change in the stacking of pairs in a column appears for some lengths of the alkyl chain (i.e, for the pentyl chains in hexaesters) in relative agreement with experimental results.

22.1-08 X-RAY PHOTOGRAPHIC STUDIES OF HAB LIQUID CRYSTALS.

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Crystals of 4,4'-diheptyloxy-azoxybenzol (HAB) in solid and liquid state were investigated by X-ray photographic Laue method. The sample was kept in a beryllium container and placed inside a copper block heater. The temperature of the sample was stabilized automatically with an accuracy of about 0.2°C. Investigations were made without and with magnetic field of intensity up to 5.5 kGs in the range of temperatures from 20°C to 125°C. The phase diagram of HAB crystals is:

$$K \xrightarrow{73^\circ} S_C \xrightarrow{94^\circ} N \xrightarrow{124^\circ} I$$

We have found that the magnetic field over 1 kGs does not exert a visible influence on the degree of order of the long axes of the molecules. In the nematic phase in the range from 93°C to 123°C the skew cybotactic groups are present. The tilt angle of the N_{SC}-groups depends on temperature according to the formula:

$$\theta_m \sim (T_o - T)^{1/2}$$

22.2-01 UNIFIED KINEMATIC THEORY OF DIFFRACTION AND DISORDERED STRUCTURES.

By S.N. Bagchi, Department of Physics, Concordia University, Montreal, Canada.

In order to obtain unequivocal results from the analysis of diffraction patterns it is essential to start from the unified theory valid for matter of any kind (S.N. Bagchi Advances in Physics (1970), 19, 119). Only this comprehensive theory can lead us to reliable simplifying assumptions often needed in practice. The fundamental concepts of "generalized" lattice and aggregates of lattices (clusters) are necessary to comprehend from a single perspective the diverse nature of the diffraction diagrams.

Our information about the structure of liquids is usually obtained from the analysis of their radial distribution functions (RDF). RDF is proportional to the convolution square of the density. Hence the conventional method of analysis of RDF is both mathematically and physically wrong. The curve fitting method of analysis, (S.N. Bagchi Acta Cryst (1972), A28, 560), based on this unified theory can yield much more reliable detailed structural parameters of the liquid state.

In the analysis of amorphous structures and noncrystalline biological structures giving rise to continuous small angle scattering there is no other satisfactory method than to deconvolute the Q-function from its edge, (S.N. Bagchi, Fourth Int. Biophysics Congress, Moscow, (1972), 755), in order to obtain unequivocal results.

For any structure the analysis of the Q-function permits us to obtain the density distribution directly from the intensity data alone. For distorted structures this would need careful quantitative analysis of the background scattering. Specialists dealing with amorphous structures ought to pay particular attention to this aspect of diffraction diagrams, very often ignored, if they desire to obtain reliable results.