22.1-1 MOLECULAR PACKING IN MESOGENIC CRYSTALS by R. F. Bryan, Department of Chemistry, University of Virginia, Charlottesville, Virginia 22901, U.S.A.

Aspects of molecular packing in crystals of homologous series of thermal mesogens are examined in relation to the type of liquidcrystalline or plastic-crystalline behavior shown by these compounds. The series examined are the p-n-alkoxybenzoic and p-nalkoxycinnamic acids, and the p-nitrophenyl-p'-n-alkoxybenzoates, which yield liquid-crystalline phases; and the polychlorinated ferrocenes, which show an alternation between normal melting and plastic-crystalline behavior dependent on their chlorine content.

The liquid crystal series show the sequence of phase transitions:

$$Crystal \to \left(S_A\right) \text{ or } \left(S_C\right) \to \left(N\right) \to Isotropic$$

Compounds in these series that do not yield liquid-crystalline phases have high packing efficiencies in the solid phase. Compounds yielding only a nematic phase have low packing efficiency deriving from steric incompatibilities between the aliphatic and aromatic components of the molecules. An anomalous instance of monotropic nematic behavior is shown to be associated with a particular crystal packing mode. Compounds yielding smectic phases all show some form of packing with two- or three-dimensional arrangements involving segregation of cores and chains.

In the chlorinated ferrocenes, the observed structures all show packing modes in which the ferrocene molecules are arranged in stacks. Those members showing plastic-crystalline behavior have a net dipole moment normal to the stack axis, whereas those showing normal melting have a zero dipole normal to that axis.

22.1-2 X-RAY DIFFRACTION STUDY OF CHOLESTEROL-CHOLESTERYL OLEATE BINARY MIXTURES. By B. Dubini, P. Mariani, <u>M.G. Ponzi-Bossi</u> and F. Rustichelli, Istituto di Fisica Medica, Facoltà di Medicina e Chirurgia, Università di Ancona, Italy, and S. Melone, Dipartimento Scienze dei Materiali e della Terra, Facoltà di Ingegneria, Università di Ancona, Italy.

The phase transitions for binary mixtures of cholesteryl oleate (CO) and cholesterol (CH) have been investigated by X-ray diffraction, differential scanning calorimetry and optical microscopy. The phase diagrams on heating involving the solid-solid and solid-isotropic liquid transitions and on cooling involving the cholesteric and smectic mesophases have been derived. In particular a strong supercooling effect of liquid cholesterol and a progressive decrease of the isotropic liquid-cholesteric and cholesteric-smectic transition temperatures were observed.

Moreover, some structural modifications induced in the smectic A and in the cholesteric phase by the presence of CH in CO were detected.

Finally, the dependence of intermolecular distances in the isotropic liquid phase were studied as a function of temperature and mixture composition. 22.1-3 X-RAY DIFFRACTION AND OPTICAL STUDIES OF ORIENTED LIQUID CRYSTAL (BBBA). By P. Mandal, M. Mitra, S. Paul and R. Paul, Department of Physics, North Bengal University, Dist. Darjeeling, Pin 734430, India.

p-n-Butoxybenzylidene-p'-butylaniline (BBBA), a polymorphic Schiff's base, is a compound of much interest and a number of studies have been made on this compound by different workers. Orientational order parameters were determined by Kirov et al. from an infrared dichroism study, (Kirov, N., Simova, P., Ratajezak, H., 1980, Mol. Cryst. Liq. Cryst. 58, 299). Fujimura et al. measured the degree of orientational order by studying the NMR spectra (Fujimura, K., Kondo, S. and Takeda, M., 1981, Mol. Cryst. Liq. Cryst. <u>64</u>, 145). Goodby et al. studied the compound by optical microscopy and miscibility method (Goodby, J.W., Gray, G.W., Leadbetter, A.J. and Mazid, M.A., 1980, Liquid Crystals of one or two dimensional order, edited by W. Helfrich and G. Hepke, Springer Verlag). We have reported the results of X-ray diffraction studies and refractive index measurement of the compound. It has got the following molecular structure and transition temperatures.



 $\mathsf{K} \stackrel{\mathsf{^{\times 8^{\circ c}}}{\rightleftharpoons}}{\mathsf{S}_{\mathsf{G}}}(\mathsf{S}_{\mathsf{G}'}) \stackrel{\mathsf{^{4^{\circ c}}}{\rightleftharpoons}}{=} \mathsf{S}_{\mathsf{B}} \stackrel{\mathsf{^{45 \cdot 5^{\circ c}}}{\rightleftharpoons}}{\mathsf{S}_{\mathsf{A}}} \stackrel{\mathsf{^{59 \cdot c}}{\rightleftharpoons}}{\overset{\mathsf{^{59 \cdot c}}}} \mathsf{N}_{\mathsf{O}} \stackrel{\mathsf{^{74 \cdot c}}{\rightleftharpoons}}{\rightleftharpoons} \mathsf{I}$

Average intermolecular distances, layer spacings and apparent molecular lengths (in case of nematic) have been determined in all the three smectic and nematic phases. Orientational order parameters of the aligned sample have been determined using the X-ray diffraction data and refractive index values. The $\langle P_2 \rangle$ values determined from optical measurements agree with the Maier-Saupe theoretical values, but $\langle P_2 \rangle$ $\langle P_4 \rangle$ determined from theoretical values. Detailed discussions on this problem will be presented.