CHAPTER-VI

SUMMARY AND CONCLUSION

that magnetic field has some effect on molecular configuration. Molecular length measured by stereomodel unit shows that molecules form associations in the mesophase, a phenomenon observed frequently in mesogenic cyanocompounds[10,11].

The structure of one of the members (HCCPP) of the above series has been solved by the direct method program SIMPEL[12] (discussed in chapter IV). It is seen that bimolecular association is found to exist also in solid state. Crystal structure of HCCPP[13] shows short contacts between molecules related through centre of symmetry around (1/2,0,1/2). These short contacts suggest associated pairs of molecules bound together by weak interactions between benzenes, pyrimidines and cyano groups. Molecules related by centre of symmetry are arranged on layers in the plane (010) and the layers are stacked along b-axis. The molecules in neighbouring layers are arranged in herring-bone like pattern. The transformation from the crystalline to the smectic phase is reconstitutive type[14,15] rather than displacive.

Refractive indices have also been measured for four members of another homologous series of alkoxy cyanobiphenyl alkyl ether (nOCB for n=9 to 12). Oredr parameters have been determined from molecular polarizabilities at different temperatures. Pronounced odd-even effect[16] is exhibited in their $\langle P_2 \rangle$ values. Since all the compounds (nOCB, n=9 to 12) of this series possess smectic A phase, $\langle P_2 \rangle$ values are compared with McMillan theory[6,7]. Experimental results are discussed in details in chapter III.

In chapter V, I present X-ray diffraction study of the same compounds (nOCB, n=9 to 12) in solid phase obtained by slowly cooling the monoliquid crystal. A monoliquid crystal is a fairly homogeneous and well oriented sample of liquid crystal which is

achieved by melting a single crystal of liquid crystalline compound to the mesomorphic state without an external field. It is a disordered crystal. By raising the temperature gradually the crystal was melted to smectic phase. Since it started as a single crystal, the molecular orientation in the monoliquid crystal is expected to be the same as that of mosophase aligned by the magnetic field. Curiously enough, the photograph at this temperature did not show any prefered orientation or alignment of the molecules. This is the observation for all the compounds. The smectic melt was now cooled down to the room temperature at the rate of 0.1^{0}/minute and diffraction photograph is taken. To raise the temperature of the sample a high temperature attachment is used which was designed and fabricated by me. From these X-ray patterns odd-even effect is again exhibited at low angles. For the even members (100CB and 120CB) several sharp diffraction maxima in the form of arcs are observed in the meridional direction. For odd members (90CB and 110CB) only one pair of broad arcs is observed. Ocurrence of sharp outer ring, d value of which corresponds to intermolecular spacing, indicates the existence of lateral order of the parallel molecules. The absence of sharp diffraction spot shows that long range order of the single crystal does not exist. It is clear that this phase is significantly different from either the smectic phase or the crystalline phase. Existence of the incommensurate modulated structures in the aligned liquid crystalline phase[17] suggests that the crystal structures of these compounds may be aperiodic. Structural models of 110CB and 120CB[18] based on strandard methods, do not agree with the experimental results. Structure determination of these two compounds still remains a difficult challenge. When these are solved we may get

some idea about the molecular arrangement in these solid phases.

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LIST OF PUBLICATIONS

1. Optical birefringence studies of the mesophase of CBOOA.
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3. An X-ray study of cyanophenyl pyrimidines. Part III. Crystal structure of 5-(trans-4-heptylcyclohexyl)-2- (4-cyanophenyl) pyrimidine.
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4. X-ray diffraction and optical studies of three mesogens of a homologous series of alkyl cyclohexyl cyanophenyl pyrimidine.
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1. X-ray diffraction study of ethyl cyclohexyl cyanophenyl pyrimidine.
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2. Determination of order parameter from optical birefringence for homologous series of mesomorphic compounds.
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