

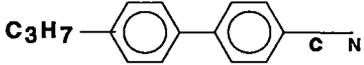
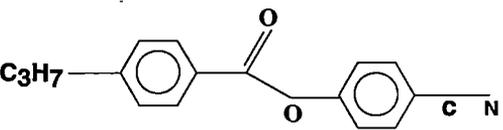
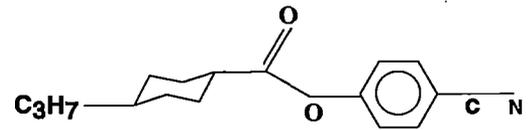
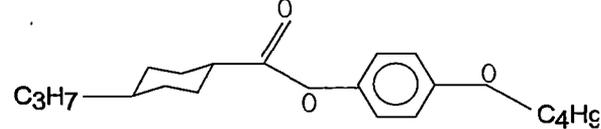
## **Chapter V**

***X-RAY AND DIELECTRIC STUDIES ON BINARY  
MIXTURES OF A CARBOXYLATE AND A  
CYANOBIPHENYL***

## 5.1 INTRODUCTION

For many years aromatic compounds based on phenyl(s) were the most common unit for liquid crystals, partly because of their easier synthesis and partly because the link between highly polarizable  $\pi$ -electron systems and mesogenicity was over-emphasized. Later it was realized that saturated systems are also excellent units when placed appropriately in relation to other planar or high polarizability regions of the cores or when the cores are entirely saturated [1]. Moreover, the presence of ester linking group results in an increase in flexibility of the core and its electron-withdrawn nature increases the core polarity. Since the ester group is intrinsically asymmetric, exchange of substituents attached to the ester group sometimes give rise to a notable change in liquid crystalline properties [2]. Phase behaviour of some such compounds is shown in Table 5.1. Data were collected from [3]. It is observed that 3CB exhibits monotropic nematic phase [4] but when the alkyl phenyl group is replaced by alkyl cyclohexyl group (3PCH) enantiotropic nematic phase sets in [5]. When both the phenyl groups are replaced by cyclohexyl groups (CCH3) stability of nematic phase is doubled and smectic phases appear while cooling [6]. On the other hand if an ester linkage group is introduced between the phenyl groups (CPPB) [7] situation does not change much from 3CB. Replacement of the phenyl by the cyclohexyl group in addition (CPPCC) increases the thermal stability of nematic phase [8]. When the highly polar cyano group is changed by a less polar and more flexible butoxy group (BPPCC) [8] thermal stability of the enantiotropic nematic is increased by about four fold compared to 3CB. Increment of number of carbon atoms by two at the cyclohexyl end and one at the butoxy end (PPPCC) results in both cybotactic and ordinary nematic phase as well as a smectic phase [8]. In this context X-ray diffraction studies were made on CPPCC and its next homologue CPBCC as well as on the above BPPCC and PPPCC; measurement of density, refractive indices, magnetic susceptibility anisotropy and elastic constants were also made by co-worker [9]. To see the effect of BPPCC guest molecules in the host 2CB matrix, binary mixtures of three different

**TABLE 5.1.**  
**Phase behaviour of some structurally related compounds**  
**(Temperatures in °C).**

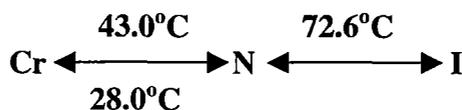
<b>3CB</b>		<b>Cr 67 N (25.5) I</b>
<b>3PCH</b>		<b>Cr 35.7 N 46 I</b>
<b>CCH3</b>		<b>Cr 58 Sm (18) Sm (44) Sm (57) N 80 I</b>
<b>CPPB</b>		<b>Cr 100 N (46) I</b>
<b>CPPCC</b>		<b>Cr 54.5(47) N 70 I</b>
<b>BPPCC</b>		<b>Cr 43(28) N 72 I</b>

concentrations have been studied by optical microscopy, X-ray diffraction technique and by static dielectric constants measurements. These results are presented in this chapter. Crystal and molecular structures of BPPCC and 2CB have also been determined by single crystal diffractometry to study the influence of molecular arrangement in the crystalline state on the phase behaviour of the mesomorphic state. These results have been described in subsequent chapters.

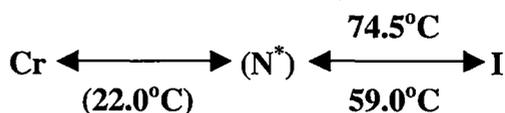
## RESULTS AND DISCUSSIONS

Transition temperatures of the pure components determined by texture studies are given below.

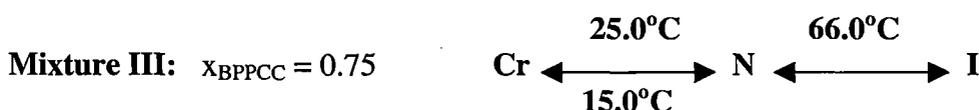
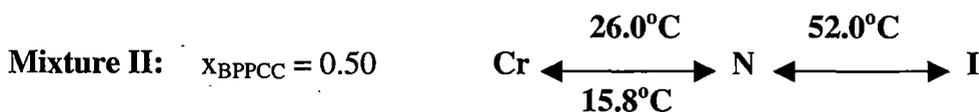
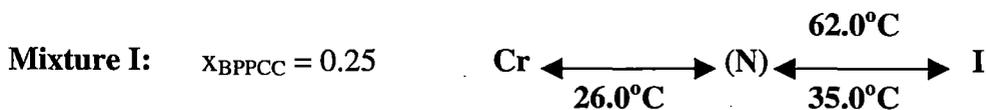
I. p-butoxyphenyl *trans*-4-propyl cyclhexane carboxylate (**BPPCC** in short)



II. 4-n-Ethyl-4'-cyanobiphenyl (**2CB** in short)

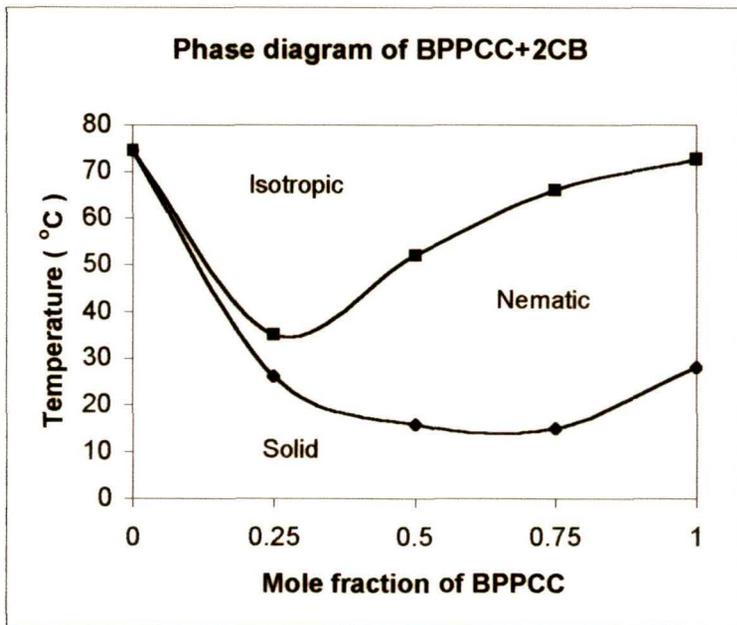


Three mixtures were prepared with 0.25, 0.5 and 0.75 of mole fraction (x) of BPPCC. By agitating the heated mixture in the isotropic phase for at least 24 hours formation of homogeneous mixture was ensured. Observed transition temperatures are as follows:

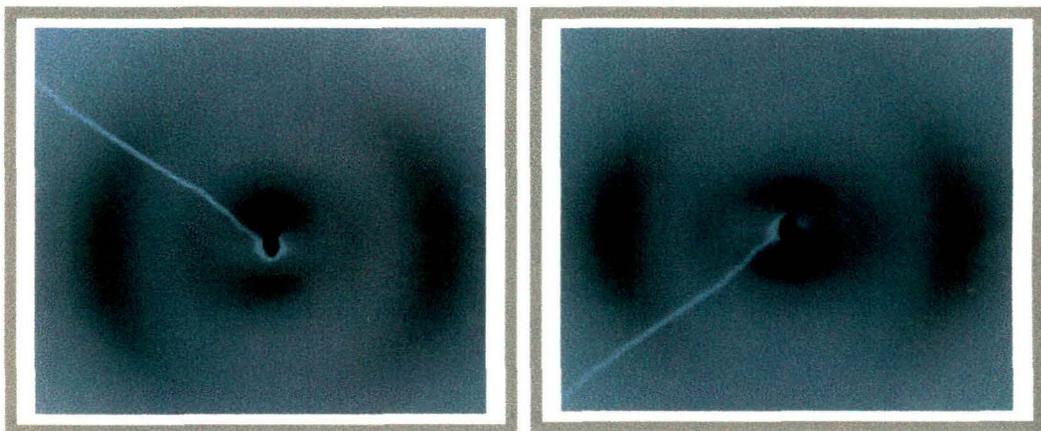


In all cases, with crossed polarizers, marble texture was observed in the nematic phase. The compound **2CB**, according to BDH literature, shows only virtual nematic phase at  $22.0^\circ\text{C}$  ( i.e. nematic transition temperature is obtained by

extrapolation of data from mixtures with other nematogens). In **Mixture I**, where only 25% **2CB** molecules are replaced by **BPPCC** molecules, the melting point drops down to 62.0°C and monotropic nematic phase is observed within 26-35°C. However, replacement of 50% or more **2CB** molecules by **BPPCC** molecules (**Mixture II and III**) results in enantiotropic nematic phase. Thermal stability of



**Figure 5.1** Phase diagram of BPPCC+2CB mixture



**Figure 5.2** X-ray diffraction photographs in nematic phase of (a) the mixture with  $x_{\text{BPPCC}}=0.50$  at 45°C and (b) the mixture with  $x_{\text{BPPCC}}=0.75$  at 26°C.

N phase in **Mixture III** is increased by about 17°C from that of pure **BPPCC**. Thus the **Mixtures II and III**, being nematic at ambient temperature because of the supercooling effect and having ranges respectively 36° and 51°, are expected to be useful in commercial display devices. The phase diagram of the mixtures is shown in Figure 5.1. Smectic A<sub>d</sub> phase was found to induce in a binary mixture (ME60.5 + 5CB, an ester/biphenyl mixture) in some compositions [10], no such phenomenon is observed in this case though the gross molecular structures are similar.

X-ray diffraction photographs confirmed the presence of ordinary nematic phase in all cases. No cybotactic nematic phase is observed in this case though one homologue (PPPCC) of BPPCC exhibits such phase [9]. Two representative magnetically aligned photographs, one each of **Mixture II** and **Mixture III**, have been presented in Figure 5.2. However, in **Mixture I**, no aligned N phase photograph could be recorded even after several attempts. But optical textures indicated that the phase is nematic and dielectric measurements confirmed that the phase is anisotropic. Therefore only **Mixture II** and **Mixture III** have been studied in detail by X-ray scattering technique. X-ray photographs were taken throughout the mesomorphic range, however, it was not possible to take photographs in the supercooling region since no arrangement for taking low temperature photographs was available.

The apparent molecular length ( $l$ ) and the average intermolecular distance ( $D$ ) over the entire mesomorphic range have been determined respectively from the low and high angle diffraction features following procedures described in Chapters II and III. These values are given in Table 5.2. Both  $l$  and  $D$  are found to increase very slowly with temperature as depicted in Figure 5.3.

Mean value of  $D$  is found to be 5.13 Å in **Mixture II** and 5.19 Å in **Mixture III** which are more than the value 5.0 Å usually found in N phase of nCB compounds [11]. Though X-ray study on **BPPCC** was done [9] previously but no  $D$  value was reported. But in two other nematogenic compounds, containing carboxylate group and lateral chloride group, the  $D$  value are found to be 5.09 Å [12]. At  $0.98T_{NI}$  on average the  $D$  value is found to be 5.09 Å for  $n=3-12$  members of the nCHBT series containing a cyclohexyl group and a -NCS group [13]. Thus it

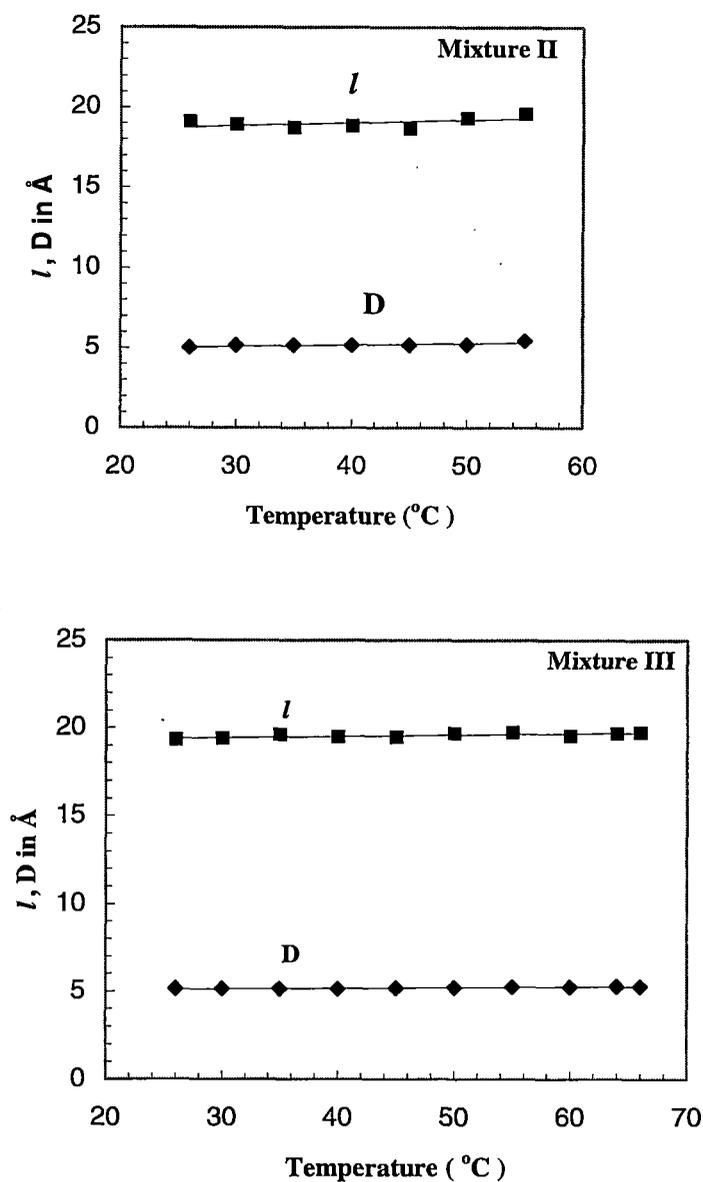


Figure 5.3 Temperature variation of *l* and D in Mixture II and Mixture III.

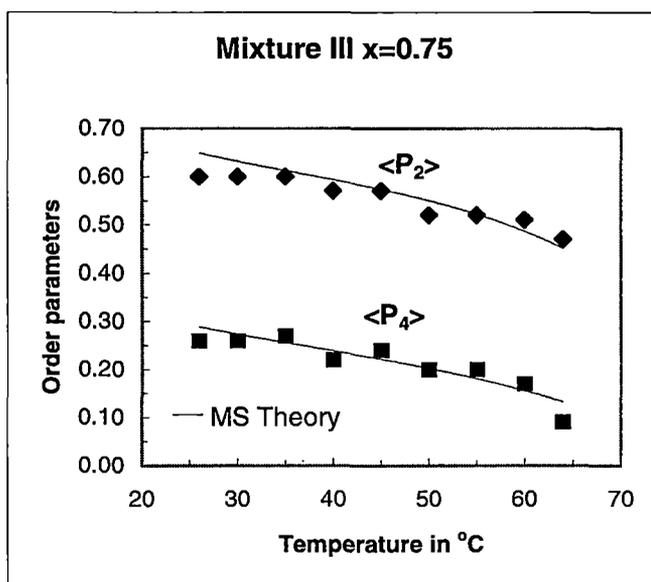
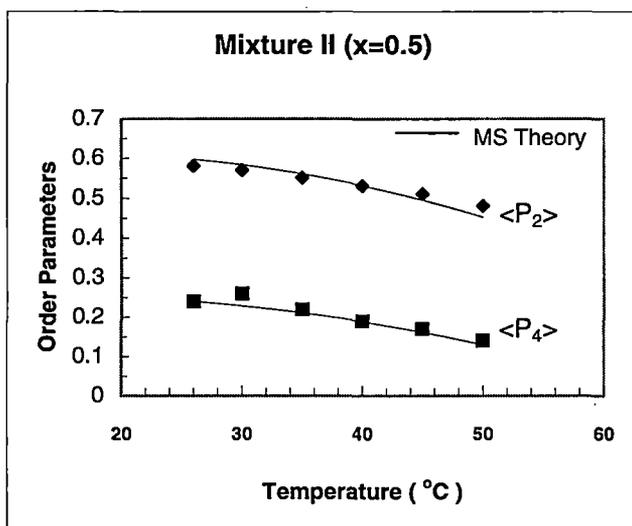
might be inferred that the packing of the dissimilar molecules in the mixtures is less efficient than that in the pure components.

The length *L*, measured from a stereo model, of **BPPCC** molecule is found to be 19.15 Å and that of molecule **2CB** is found to be 12.85 Å which have been confirmed by crystal structure analysis of the compounds (Chapter VI and VII). From simple additive rule [ $l = x_{\text{BPPCC}} \cdot L_{\text{BPPCC}} + x_{\text{2CB}} \cdot L_{\text{2CB}}$ ] one expects that the apparent lengths in **Mixture II** and **Mixture III** would be 16.0 Å and 17.58 Å.

However, the average  $l$  of the molecules is found to be 19.6 Å in both the **Mixtures**, considerably different from the expected value. In pure **BPPCC** mean value of the observed  $l$  is about 20.87 Å and  $l/L$  ratio is about 1.09 [9]. Though for pure **2CB** this data is not available but for many homologues of the nCB series it is observed [11] that  $l/L$  ratio is about 1.4. Even cyanocompounds with ester linkage group (CPPCC and CPBCC) showed similar result [9]. In both cases it is assumed that existence some sort of bimolecular association is the cause of  $l/L$  greater than 1. In BPPCC the molecules of the pair are in almost complete overlap configuration whereas in nCB molecules the extent of overlap is much less. If the associated length of the pairs is taken as the effective lengths of the molecules within nematic phase, then the calculated  $l$  values in the mixtures become 20.15 Å and 19.43 Å respectively, very close to the observed value (19.6 Å). Thus bimolecular association within same type of molecules (homo dimmers) is likely to be present in the mixtures as well. In a binary mixture of dodecyloxy cyanobiphenyl and a four-ring carboxylate molecule, where both the molecules have strong axial dipole moments and much longer molecular lengths [ $L_{12OCB}=26.0$  Å and  $L_{7CBB}=31.5$  Å], both homo- and hetero- dimmers are found to be present [14].

Orientational order parameters,  $\langle P_2 \rangle$  and  $\langle P_4 \rangle$ , have been determined from the intensity distribution of the outer halo of the X-ray photographs following the procedure described in Chapters II and III. Order parameter values are given in Tables 5.3-5.4. Variation of the order parameters with temperature is shown in Figure 5.4. It is observed that for both the mixtures order parameters  $\langle P_2 \rangle$  and  $\langle P_4 \rangle$  agree well with the values predicted by Maier-Saupe theory. Only for the **Mixture III** at low temperature region  $\langle P_2 \rangle$  values are lower than MS values. Moreover, in this system the molecules are found to be less ordered than in systems described in previous two chapters. However, the molecules of the previous systems are longer and less rigid than the present molecules and therefore, expected to be less ordered.

For pure BPPCC, observed  $\langle P_2 \rangle$  and  $\langle P_4 \rangle$  values [9] are also found to be consistent with MS theory and in the mixtures no significant change in order parameters is observed. For example,  $\langle P_2 \rangle$  and  $\langle P_4 \rangle$  values at  $(T_{NI} - 12)^\circ\text{C}$  are



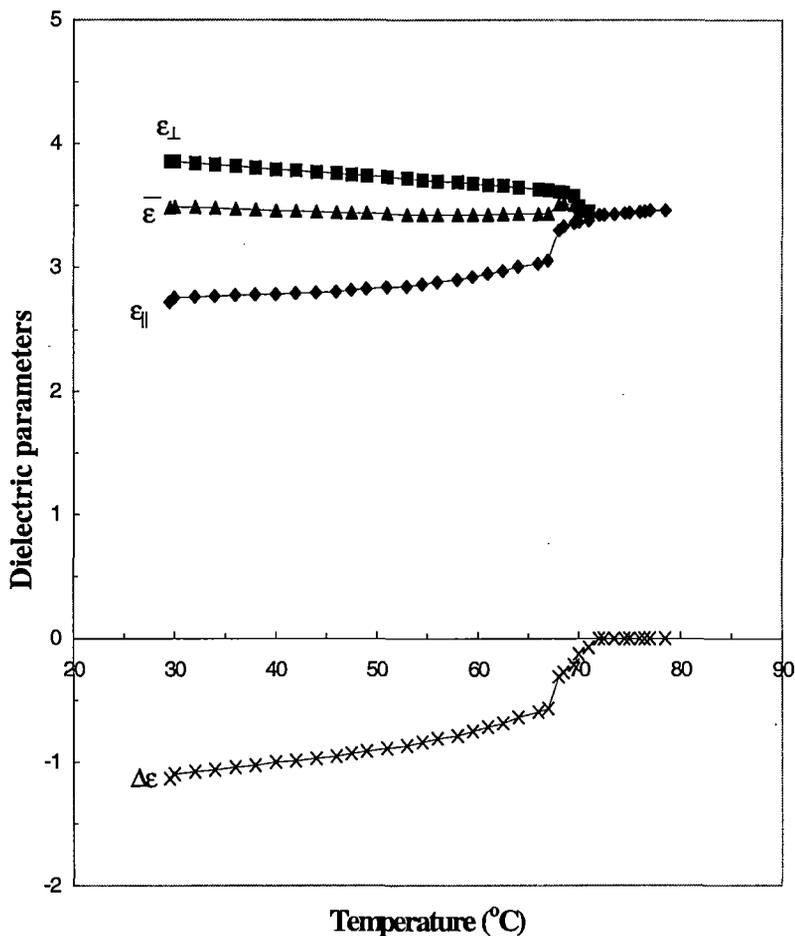
**Figure 5.4** Orientational order parameters of Mixture II and Mixture III

found to be (0.53, 0.19), (0.52, 0.20) and (0.54, 0.18) respectively in **Mixture II**, **Mixture III** and **BPPCC**.

Static dielectric permittivities,  $\epsilon_{\parallel}$  and  $\epsilon_{\perp}$ , have been measured parallel and perpendicular to the molecular axis following the procedure described in Chapter II.

Using cells made of ITO coated conducting glass plates dielectric parameters were measured at 10 KHz by an LCR bridge. Magnetic field of about 5 KGauss was applied to align the samples in homeotropic (for  $\epsilon_{\parallel}$  measurement) and homogeneous (for  $\epsilon_{\perp}$  measurement) geometry. Average permittivity  $\bar{\epsilon}$  and the anisotropy in permittivities  $\Delta\epsilon$  have also been calculated. Since no dielectric data for **BPPCC** was reported earlier dielectric measurements have been made on pure **BPPCC** as well. Values of the dielectric parameters,  $\epsilon_{\parallel}$ ,  $\epsilon_{\perp}$ ,  $\bar{\epsilon}$  and  $\Delta\epsilon$ , are collected in Table 5.5 for **BPPCC** and in Tables 5.6-5.8 for all three mixtures. Variations of dielectric parameters have been shown in Figures 5.5-5.6. The compound **BPPCC** shows small ( $\Delta\epsilon=-1.1$  at  $29.5^{\circ}\text{C}$ ) but negative anisotropy because of the presence of non-axial dipole moment of the ester group in the molecule.  $\Delta\epsilon=-1.26$ ,  $-1.20$  and  $-1.05$  (at low end of nematic range) have been reported for the homologues **EPPCC**, **EPBCC** and **MPBCC** of the **BPPCC** series [15]. However, all the three mixtures show large positive anisotropy. Since **2CB** is only virtually nematic no mesophase data for **2CB** is available. All members of the **nCB** series show large positive dielectric anisotropy, for example  $\Delta\epsilon=8.0$  for **8CB** at  $0.98T_{\text{NI}}$  [13]. Thus the dielectric behaviour of the mixtures is dominated by the **2CB** component. Even when only 25% of the **BPPCC** molecules are replaced by the **2CB** molecules (Mixture III) substantial positive anisotropy (maximum value is about 2.73) is yielded. Replacement of 50% and 75% **BPPCC** molecules by **2CB** molecules results in larger  $\Delta\epsilon$ .

In all the **mixtures** dielectric permittivity in the isotropic phase  $\epsilon_{\text{iso}}$  is found, from the above figures, to be larger than  $\bar{\epsilon}$  in the nematic phase, no such jump is observed in **BPPCC**. These suggest presence of some sort of anti-parallel dipolar association within nematic phase of the mixtures. This dipolar association breaks down completely or partially in the isotropic phase resulting in increased effective dipole moment of the molecules and thereby increased permittivity. In **BPPCC** probably no such change of molecular associations takes place during the **N-I** transition, though from X-ray study anti-parallel dipolar association is found to exist in **N** phase.



**Figure 5.5** Temperature variation of dielectric parameters of BPPCC.

It is also observed that in pure BPPCC the values of  $\epsilon_{\perp}$  decrease very slowly with temperature while  $\epsilon_{\parallel}$  and  $\Delta\epsilon$  values are found to increase very slowly. In the mixtures, however,  $\epsilon_{\parallel}$  and  $\Delta\epsilon$  values are found to decrease with temperature as expected for a Debye type liquid.

It is also clear from the graphs that all the dielectric parameters are substantially higher in the **mixtures** than that in pure **BPPCC** suggesting, as noted earlier, that dielectric behaviour of the mixtures is dominated by the strongly axial polar component 2CB.

Using the expressions for  $\epsilon_{\parallel}$  and  $\epsilon_{\perp}$  of Maier and Meier [Equations 2.24 and 2.25], which were obtained by extending Onsager's theory of isotropic liquid to

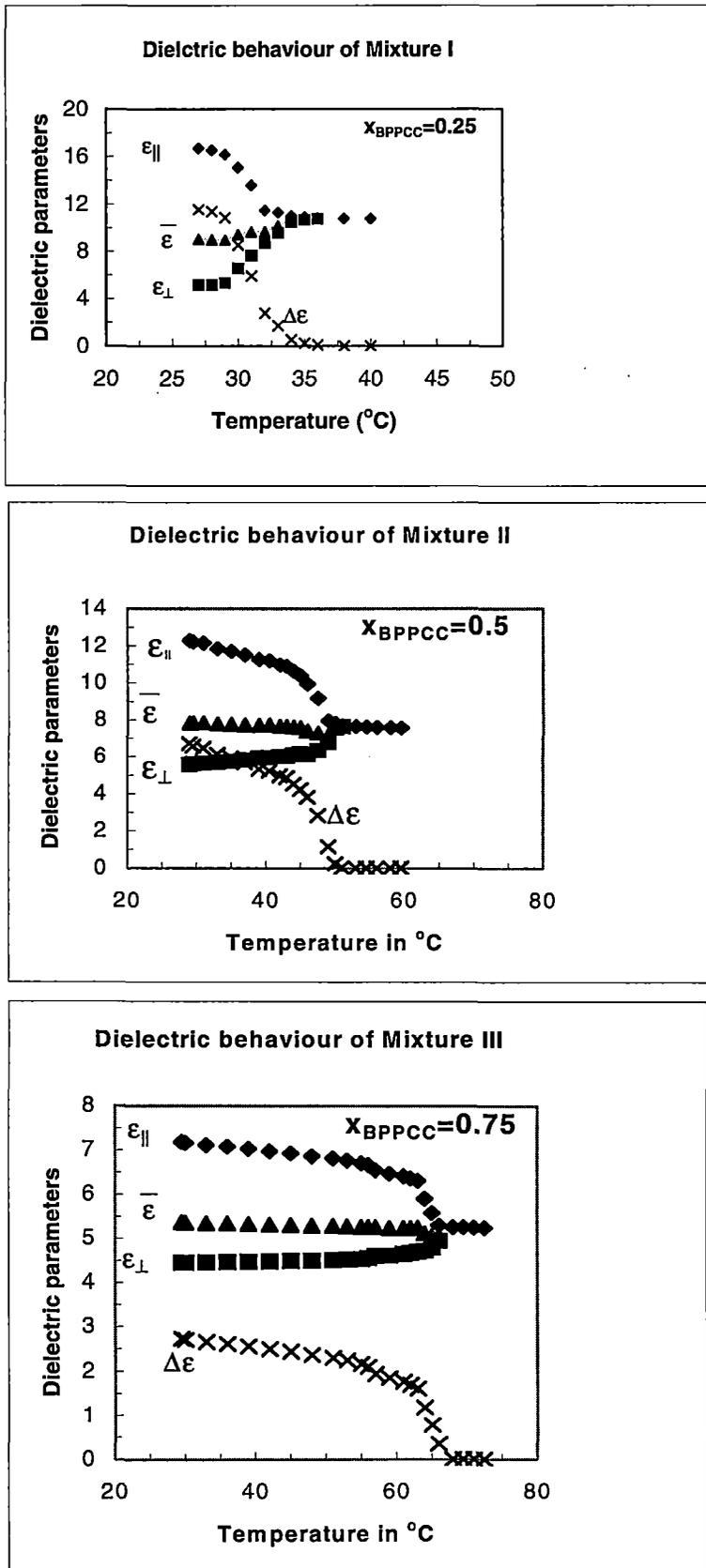


Figure 5.6 Temperature variation of dielectric parameters of the mixtures.

nematics, effective value of the dipole moment  $\mu$  and the angle  $\beta$  which it makes with the molecular long axis are calculated at various temperatures for BPPCC. The calculation procedure has been described in detail in Chapter II. Mean field order parameters  $\langle P_2 \rangle$  and densities, average molecular polarizability and polarizability anisotropy values [9] estimated from refractive indices using Neugebauer's method [16] were used in this calculation. Since the above data were not available for the mixtures and we could not determine those values for want of sufficient sample,  $\mu$  and  $\beta$  could not be calculated for the mixtures. Calculated values of  $\mu$  and  $\beta$  have been given in Table 5.9. Both are found to increase slowly with temperature except near  $T_{NI}$ . Dipole moment of the free BPPCC molecules is not available but for few homologues of the series (with  $C_1$  or  $C_2$  at the alkoxy end and  $C_3$  or  $C_5$  at the alkyl end) reported  $\mu$  values are 2.08D, 2.17D and 2.23D [15]. It was also shown previously for nCB series that free molecule dipole moment does not vary appreciably with chain length [17,18]. Therefore, it may be reasonably assumed that the free molecule dipole moment of BPPCC will be around 2.15 Debye. Effective value of the dipole moment within nematic phase is, therefore, about 20% less than the above free molecule value, again suggesting the presence of antiferroelectric type short range order between the neighbouring molecules. This type of result has also been tried to explain assuming the presence of both monomer and dimer molecules [10, 19-22]. Moreover, it is observed that the effective dipole moment is at large angle ( $\beta_{min}=74.6^\circ$  and  $\beta_{max}=83.9^\circ$ ) with the molecular long axis and BPPCC molecules, therefore, exhibit negative dielectric anisotropy. Kali *et al.* [15] reported that the value of  $\beta$ , calculated from the known group dipole moments [23], is about  $72^\circ$  in the lower homologues. Thus observed low temperature  $\beta$  value agrees reasonably well with this data. However, it is observed that the calculated  $\beta$  values increase by  $1-2^\circ$  if  $\langle P_2 \rangle$  determined from refractive indices data are used in the calculation instead of MS  $\langle P_2 \rangle$  values, though this produces no change in the values of  $\mu$ .

A quantitative measure of the above dipolar correlation is possible to determine using Bordewijk [24] theory of anisotropic dielectrics which is an

extension of Kirkwood-Fröhlich theory [25] where, unlike Maier-Meier theory, short range dipole-dipole interaction was considered explicitly. Correlation factor ( $g_\lambda$ ), called Kirkwood correlation factor, are calculated taking into account the correlation between neighbouring dipole moments only where the suffix  $\lambda$  refers to  $\parallel$  and  $\perp$  to the nematic director. The ensemble average of the  $\parallel$  and  $\perp$  components of the molecular dipole moments were calculated following the procedure of Bata and Buka [26] and has been described in detail in Chapter II. Obviously,  $g_\lambda = 1$  signifies no correlation (monomeric system),  $g_\lambda = 0$  means perfect antiparallel correlation and  $g_\lambda = 2$  means perfect parallel correlation. Calculated values are shown in Table 5.9. Values of  $g_\parallel$  is found to be 0.35 and 0.83 at the low and high temperature end of the nematic phase while corresponding values of  $g_\perp$  are 1.15 and 1.17. These values suggest parallel components of the molecular dipole moments are strongly correlated in antiferroelectric fashion at low temperatures but at high temperatures this correlation is almost negligible. Over the entire nematic range the correlation of the perpendicular component is ferroelectric type but almost negligible. No such data are available for BPPCC or its homologues. However, in a nematogenic compound, containing two carboxylate groups, moderate  $g_\parallel$  but similar  $g_\perp$  values were observed [27].

In the isotropic phase, the effective dipole moment was calculated by Kirkwood-Fröhlich relation [25] and found to be 1.87 Debye at 73.0°C. Corresponding dipole correlation factor ( $g_{iso}$ ) is 0.76. Thus antiparallel dipolar correlation is found to exist even in the isotropic phase. It is also observed that  $\mu$  value does not change appreciably at  $T_{NI}$ , similar phenomenon was noticed earlier while comparing the values of  $\epsilon_{iso}$  and  $\bar{\epsilon}$  below  $T_{NI}$ . Thus X-ray and dielectric study suggests the presence of anti-parallel molecular association in **BPPCC** in both nematic and isotropic phases and no effective change in molecular associations takes place during the **N-I** transition.

Since the threshold voltage and other operational parameters of liquid crystal display devices depend on  $\Delta\epsilon$  and since the multiplexability of matrix displays may be limited by the temperature dependence of  $\Delta\epsilon$  and since multicomponent mixtures

are used in commercial display devices, the results presented above on pure compound and mixtures are of interest from application point of view in addition to the general interest of understanding the basic science.

**TABLE 5.2**

**D and *l* values at different temperatures**

Mixture II			Mixture III		
Temp.(°C)	D (Å)	<i>l</i> (Å)	Temp.(°C)	D (Å)	<i>l</i> (Å)
26	4.99	19.1	26	5.12	19.3
30	5.16	18.9	30	5.14	19.4
35	5.14	18.7	35	5.15	19.6
40	5.15	18.9	40	5.14	19.5
45	5.16	18.7	45	5.18	19.5
50	5.19	19.3	50	5.2	19.7
55	5.44	19.6	55	5.25	19.8
			60	5.23	19.5
			64	5.29	19.7
			66	5.3	19.8

**TABLE 5.3**  
**Orientational order parameters of Mixture II**

Temperature (°C)	$\langle P_2 \rangle$	$\langle P_4 \rangle$	MS Value	
			$\langle P_2 \rangle$	$\langle P_4 \rangle$
26	0.58	0.24	0.60	0.24
30	0.57	0.26	0.58	0.23
35	0.55	0.22	0.56	0.21
40	0.53	0.19	0.53	0.19
45	0.51	0.17	0.50	0.16
50	0.48	0.14	0.45	0.13

**TABLE 5.4**  
**Orientational order parameters of Mixture III**

Temperature (°C)	$\langle P_2 \rangle$	$\langle P_4 \rangle$	MS Value	
			$\langle P_2 \rangle$	$\langle P_4 \rangle$
26	0.60	0.26	0.65	0.29
30	0.60	0.26	0.63	0.27
35	0.60	0.27	0.61	0.26
40	0.57	0.22	0.60	0.24
45	0.57	0.24	0.57	0.22
50	0.52	0.20	0.55	0.20
55	0.52	0.20	0.52	0.18
60	0.51	0.17	0.49	0.16
64	0.47	0.09	0.45	0.13

**TABLE 5.5**  
**Dielectric parameters for BPPCC**

<b>BPPCC</b>				
<b>Temp.(°C)</b>	$\epsilon_{\parallel}$	$\epsilon_{\perp}$	$\bar{\epsilon}$	$\Delta\epsilon$
71	3.380	3.451	3.427	-0.071
70	3.368	3.493	3.451	-0.125
69.5	3.362	3.576	3.504	-0.214
68.5	3.332	3.605	3.514	-0.273
68	3.303	3.611	3.508	-0.309
67	3.053	3.623	3.433	-0.570
66	3.030	3.629	3.429	-0.599
64	3.006	3.647	3.433	-0.641
62.5	2.970	3.659	3.429	-0.688
61	2.947	3.665	3.425	-0.718
59.5	2.923	3.676	3.425	-0.754
58	2.899	3.688	3.425	-0.789
56	2.881	3.694	3.423	-0.813
54.5	2.863	3.706	3.425	-0.843
53	2.846	3.718	3.427	-0.872
51	2.840	3.730	3.433	-0.890
49	2.828	3.742	3.437	-0.914
47.5	2.816	3.748	3.437	-0.932
46	2.804	3.760	3.441	-0.955
44	2.798	3.771	3.447	-0.973
42	2.792	3.783	3.453	-0.991
40	2.786	3.789	3.455	-1.003
38	2.780	3.807	3.465	-1.027
36	2.774	3.819	3.471	-1.044
34	2.769	3.831	3.477	-1.062
32	2.763	3.843	3.483	-1.080
30	2.757	3.855	3.489	-1.098
29.5	2.721	3.855	3.477	-1.134

**TABLE 5.6**  
**Dielectric parameters for Mixture I**

<b>Mixture I</b>				
<b>Temp.(°C)</b>	$\epsilon_{\parallel}$	$\epsilon_{\perp}$	$\bar{\epsilon}$	$\Delta\epsilon$
36	10.828	10.739	10.768	0.089
35	10.887	10.656	10.733	0.231
34	10.988	10.454	10.632	0.534
33	11.285	9.581	10.149	1.703
32	11.463	8.709	9.627	2.754
31	13.552	7.647	9.615	5.905
30	15.065	6.543	9.384	8.522
29	16.157	5.309	8.925	10.848
28	16.519	5.154	8.942	11.365
27	16.661	5.142	8.982	11.519

**TABLE 5.7**  
**Dielectric parameters for Mixture II**

<b>Mixture II</b>				
<b>Temp.(°C)</b>	$\epsilon_{\parallel}$	$\epsilon_{\perp}$	$\bar{\epsilon}$	$\Delta\epsilon$
51	7.670	7.635	7.647	0.036
50	7.801	7.564	7.643	0.237
49	7.949	6.792	7.178	1.157
47.5	9.166	6.347	7.287	2.819
46	9.937	6.127	7.397	3.810
45	10.383	6.169	7.574	4.214
44	10.626	6.110	7.615	4.516
43	10.887	6.021	7.643	4.866
42	10.970	6.003	7.659	4.967
40.5	11.196	5.967	7.710	5.228
39	11.255	5.926	7.702	5.329
37	11.498	5.831	7.720	5.668
35	11.688	5.765	7.740	5.923
33	11.848	5.712	7.758	6.136
31	12.139	5.665	7.823	6.475
29.5	12.204	5.635	7.825	6.570
29	12.276	5.576	7.809	6.700

**TABLE 5.8**  
**Dielectric parameters for Mixture III**

<b>Mixture III</b>				
<b>Temp.(°C)</b>	$\epsilon_{\parallel}$	$\epsilon_{\perp}$	$\bar{\epsilon}$	$\Delta\epsilon$
66	5.297	4.952	5.067	0.344
65	5.576	4.798	5.057	0.777
64	5.902	4.727	5.119	1.175
63	6.311	4.703	5.239	1.608
62	6.365	4.674	5.237	1.691
61	6.412	4.650	5.237	1.763
59	6.466	4.620	5.235	1.846
57	6.543	4.608	5.253	1.935
56	6.662	4.561	5.261	2.101
55	6.703	4.537	5.259	2.166
53	6.768	4.525	5.273	2.243
51	6.816	4.513	5.281	2.303
48	6.863	4.501	5.289	2.362
45	6.929	4.490	5.303	2.439
42	6.976	4.478	5.310	2.498
39	7.030	4.472	5.324	2.558
36	7.077	4.466	5.336	2.611
33	7.113	4.460	5.344	2.653
30	7.160	4.454	5.356	2.706
29.5	7.184	4.454	5.364	2.730

**TABLE 5.9**  
**Effective dipole moment ( $\mu$ ), angle ( $\beta$ ) and correlation factors of BPPCC**

Temperature (°C)	$\mu$	$\beta$	$g_{\parallel}$	$g_{\perp}$
43	1.73	74.6	0.35	1.15
48	1.75	75.8	0.43	1.15
51	1.76	76.6	0.5	1.16
55	1.77	78.3	0.59	1.16
60	1.8	83.2	0.83	1.16
63	1.82	83.9	0.96	1.17
68	1.9	66	0.89	1.24
70	1.86	60.5	0.83	1.17
73	1.87 iso		0.76 iso	

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