

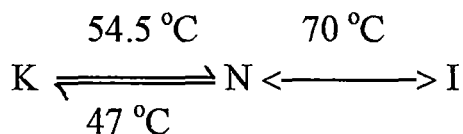
## **CHAPTER- 3**

*X-ray diffraction studies and measurement of density, refractive indices, magnetic susceptibility anisotropy, splay and bend elastic constants of four cyclohexane carboxylate compounds.*

In this chapter, I shall present experimental data on four liquid crystalline compounds. The compound studied with their chemical structures and transition temperatures are given below:

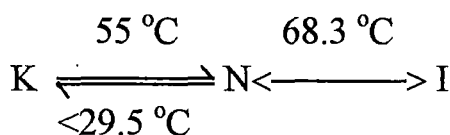
I. p-cyanophenyl trans-4-propyl cyclohexane carboxylate.

( CPPCC in short)



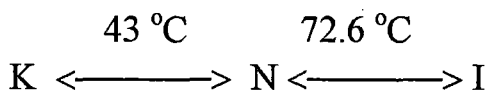
II. p-cyanophenyl trans-4-butyl cyclohexane carboxylate.

( CPBCC in short)



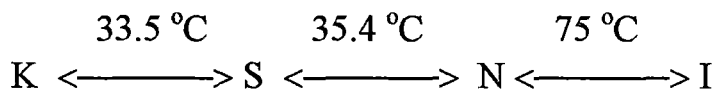
III. p-butoxyphenyl trans-4-propyl cyclohexane carboxylate.

( BPPCC in short)



IV. p-pentoxyphenyl trans-4-pentyl cyclohexane carboxylate.

( PPPCC in short)



( Ph= Phenyl ring, Cy = Cyclohexyl ring)

The transition temperatures were recorded by observing the textures under a polarising microscope using Mettler FP 80/ 82 hot stage. The transition temperatures agreed with those given in the literature [1] and the compounds were used without further purification. The physical properties studied were density, refractive index, magnetic susceptibility anisotropy, and bend and splay elastic constants. X-ray diffraction photographs of all the compounds in their mesophase were also taken. All the experiments covered the full mesomorphic temperature ranges of the substances. The respective experimental procedures have been described in detail in Chapter 2 of this thesis.

Figures 3.1- 3.4 give the temperature variation of density of CPPCC, CPBCC, BPPCC and PPPCC. For all the compounds the density decreases monotonically with increasing temperature and there is a small density change at the nematic-isotropic transition temperature. Only PPPCC has a smectic phase and it appears that the density changes continuously at the smectic to nematic transition.

The temperature variation of ordinary and extraordinary refractive indices for CPPCC, CPBCC, BPPCC and PPPCC at four different wavelengths are given in Figures 3.5 to 3.8. The density and refractive indices (at different wavelengths) of CPPCC, CPBCC and PPPCC have already been reported by Takahashi et al [2] and their values agree with our values within experimental errors. However, they have not calculated order parameters from their data, whereas we have calculated the order parameters and compared these values with those obtained from magnetic susceptibility and x-ray diffraction studies.

The values of densities, ordinary and extraordinary refractive indices at different temperatures for CPPCC, CPBCC, BPPCC and PPPCC at

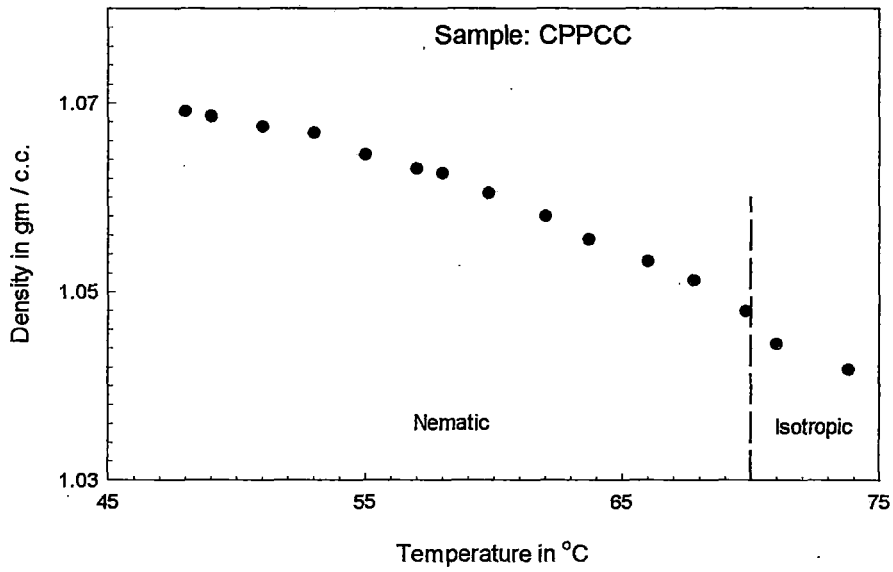


Figure 3.1. Density values as a function of temperature.

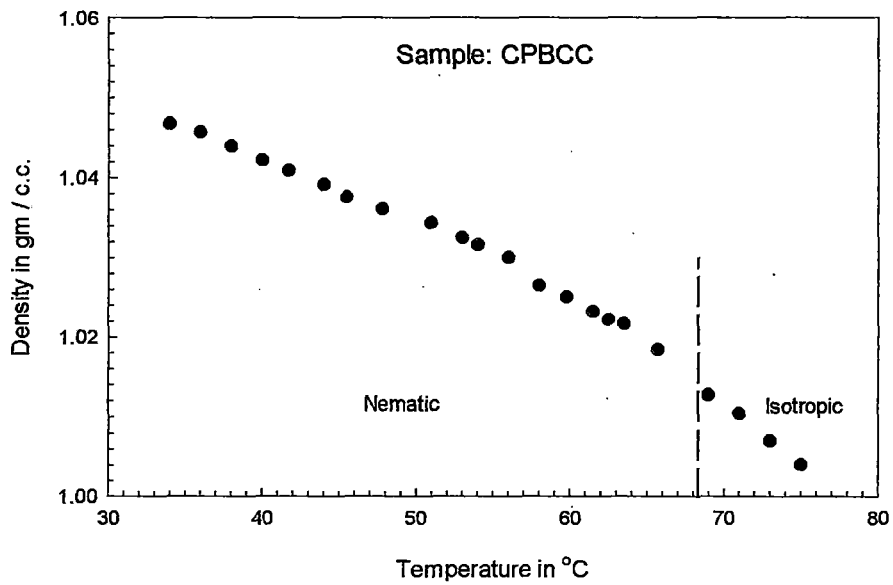


Figure 3.2. Density values as a function of temperature.

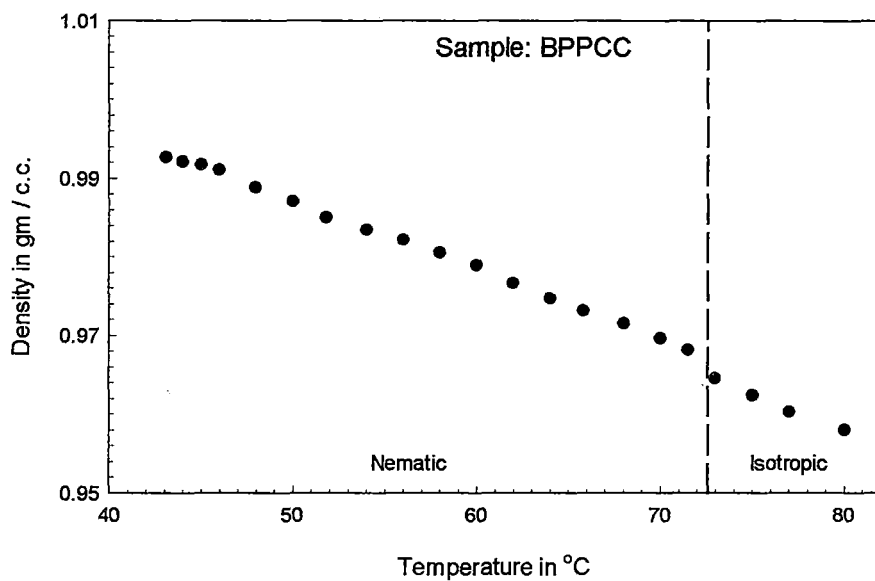


Figure 3.3. Density values as a function of temperature.

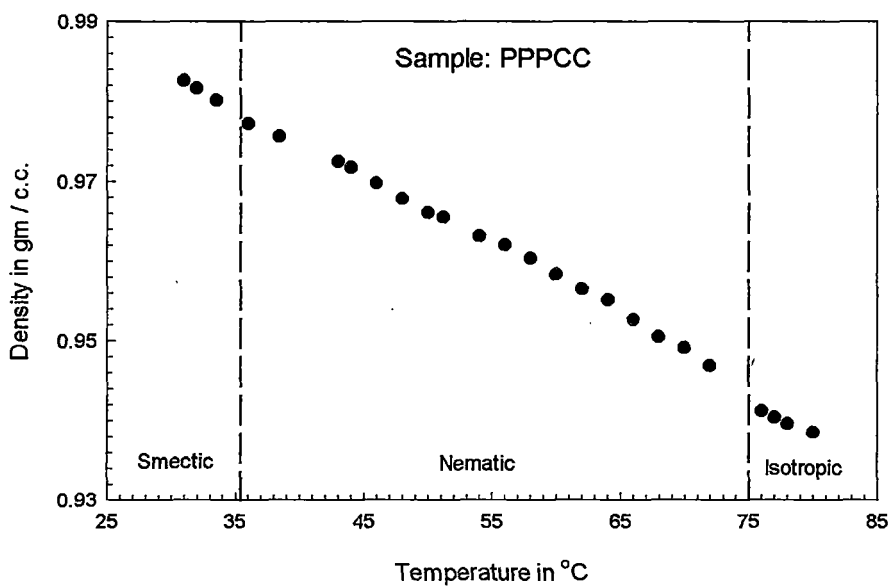


Figure 3.4. Density values as a function of temperature.

wavelengths of 4358 Å, 5461 Å, 5780 Å and 6907 Å are given in Tables 3.1 to 3.4. The respective polarisabilities calculated for these four mesogens using Vuks procedure (equation 2.24 & 2.25) are tabulated in Tables 3.5 to 3.8. The same polarisabilities calculated following Neugebauer method (equations 2.22 & 2.23) are given in Tables 3.9 to 3.12. The polarisability anisotropies in the perfectly aligned ( $\langle P_2 \rangle = 1$ ) samples have been determined by Haller's extrapolation procedure (Chapter 2) and have been given in the respective Table. The order parameters calculated using Vuks polarisability values are tabulated in Tables 3.13 to 3.16 for CPPCC, CPBCC, BPPCC and PPPCC. Finally, the order parameters of these four mesogens using Neugebauer polarisability values are given in Tables 3.17 to 3.20. Though for all the four compounds the polarisability anisotropy calculated from Vuks method are larger than those calculated from Neugebauer procedure, the order parameters from these two methods agree within  $\pm 0.01\%$ . Mitra et al [3], for some other mesogens, also observed that the Vuks and Neugebauer procedures give almost same order parameter values, though the polarisability anisotropies were different.

The x-ray diffraction photographs from the mesophases of CPPCC, CPBCC, BPPCC and PPPCC at different temperatures are shown in plates 3a-3i. The samples were aligned in a magnetic field of about 5 Kilogauss. The angular distribution of x-ray intensities (in arbitrary scale), after correction for background and conversion from optical densities to x-ray intensities, for the outer diffraction arc for CPPCC at five different temperatures are tabulated in Table 3.21. The corresponding orientational distribution functions calculated by Leadbetter method (equation 2.16) are shown in Table 3.22. Similarly Tables 3.23 and 3.24 give the x-ray intensities and distribution function respectively for CPBCC. For BPPCC

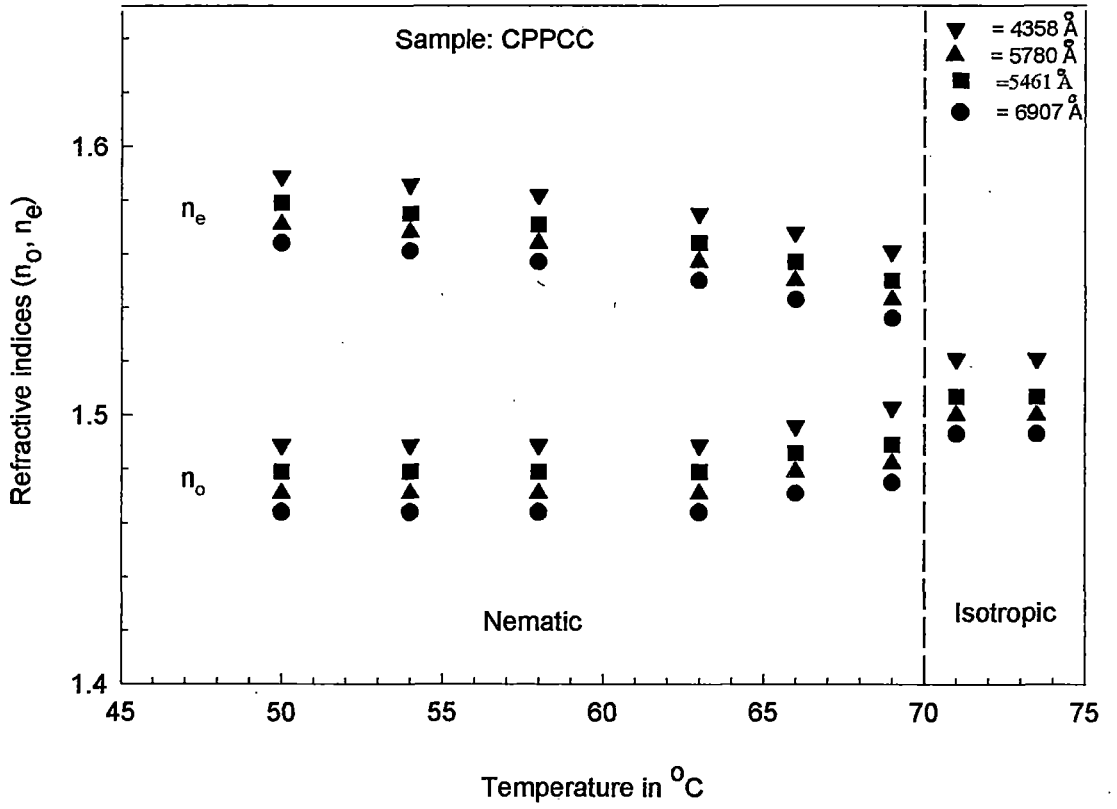


Figure 3.5. Variation of refractive indices ( $n_o, n_e$ ) with temperature.

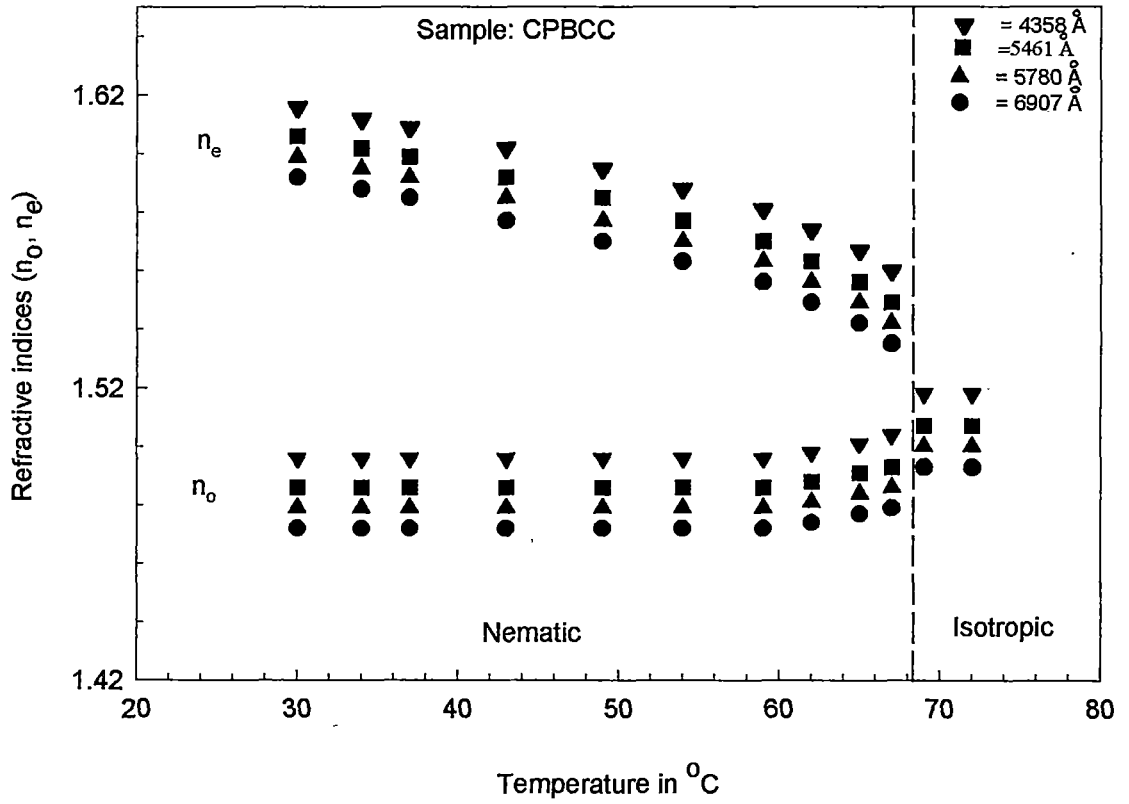


Figure 3.6. Variation of refractive indices ( $n_o, n_e$ ) with temperature.

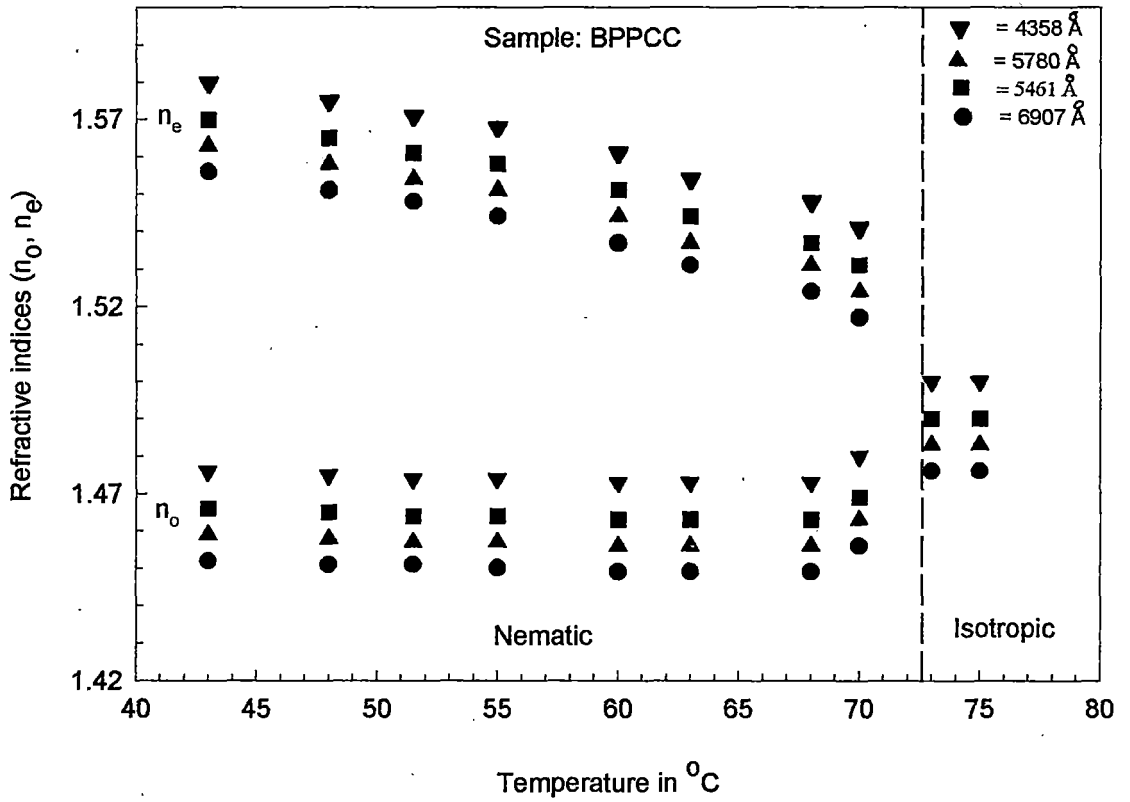


Figure 3.7. Variation of refractive indices ( $n_o, n_e$ ) with temperature.

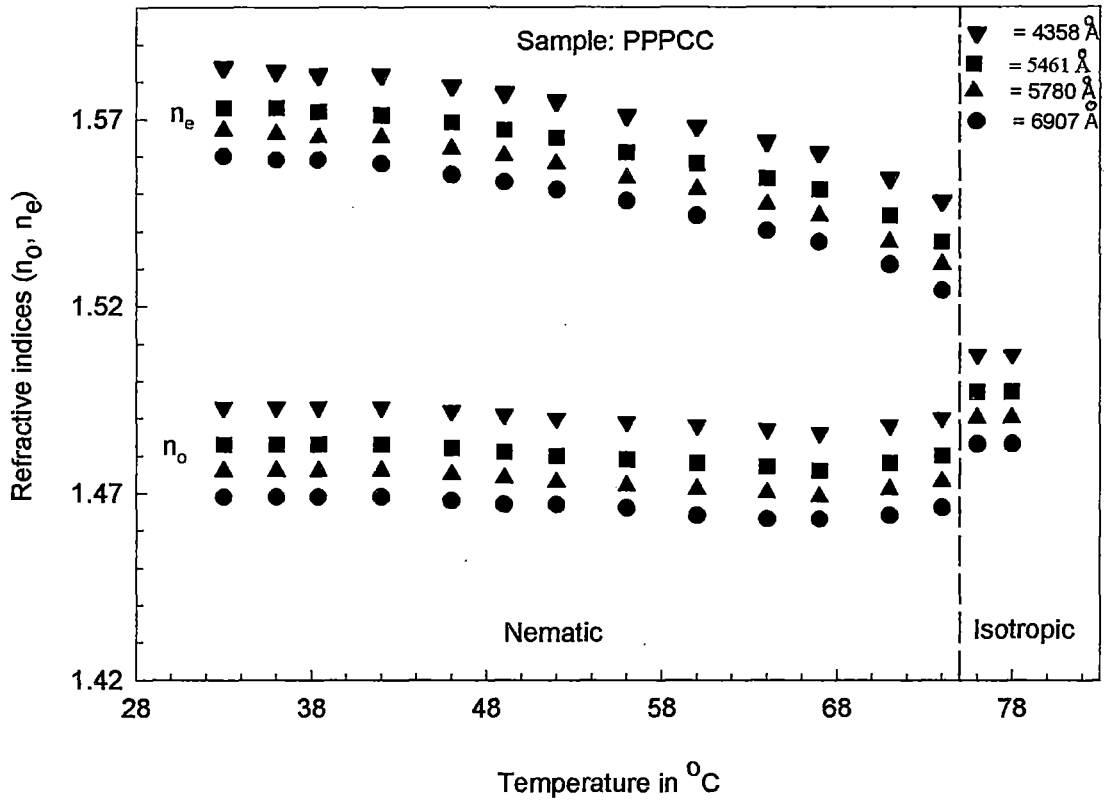


Figure 3.8. Variation of refractive indices ( $n_o, n_e$ ) with temperature.

the corresponding values are tabulated in Tables 3.25 and 3.26. Tables 3.27 and 3.28 similarly give the x-ray intensity and distribution function values for PPPCC. The orientational order parameters  $\langle P_2 \rangle$  and  $\langle P_4 \rangle$  of CPPCC, CPBCC, BPPCC and PPPCC at different temperatures are tabulated in Tables 3.29 to 3.32.

The apparent molecular lengths of CPPCC and CPBCC in the mesophase, as obtained from the inner x-ray diffraction arc are given in Table 3.33 and 3.34. Tables 3.35 and 3.36 give the corresponding apparent molecular lengths for BPPCC and PPPCC respectively. The temperature variation of the apparent molecular lengths of all the four mesogens are shown in Figure 3.9a to 3.9d. The model lengths of these molecules in their fully extended form have been determined and are noted in the respective tables. It can be seen that for the two cyano compounds (CPPCC and CPBCC) the ratio of apparent molecular lengths to their model molecular lengths are nearly 1.4, showing formation of a molecular association (dimers) in the mesophase. This is in accordance with x-ray diffraction observation on cyanobiphenyls [4], where this ratio of apparent to model molecular lengths are also about 1.4. The other two compounds have no terminal polar groups and the ratio of apparent to model molecular lengths are 1.09 and 1.15 for BPPCC and PPPCC respectively, showing that even if there are association of molecules in the mesophase of these compounds, their apparent length is almost equal to the model length of single molecule. In fact, PPPCC forms cybotactic nematic phase, that means its molecules form small smectic like clusters. It may be mentioned that in PPPCC, we have observed a smectic phase between 33.5 °C to 35.4 °C from texture studies. However, the smectic phase could not be identified from x-ray diffraction pattern (Plate 3g) since the sample could

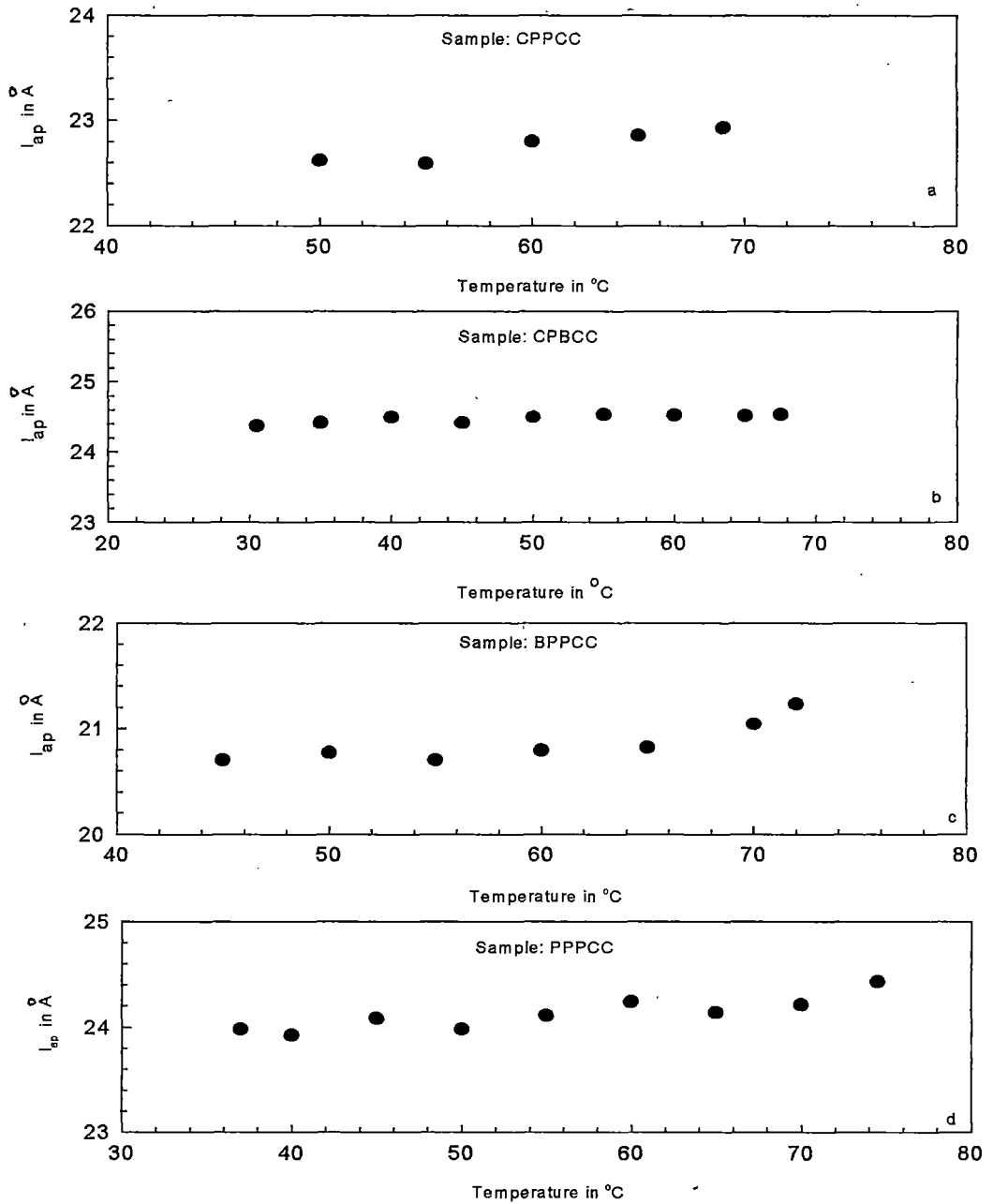


Figure ( 3.9a - 3.9d ). Temperature variation of apparent molecular length ( $l_{ap}$ ).

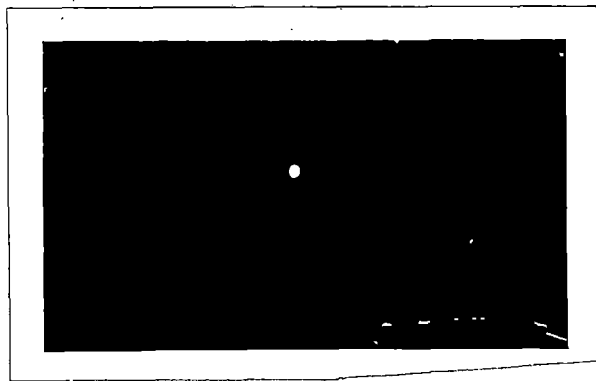


Plate 3a: X-ray diffraction photograph of the oriented sample in the nematic phase of CPPCC at 50°C.

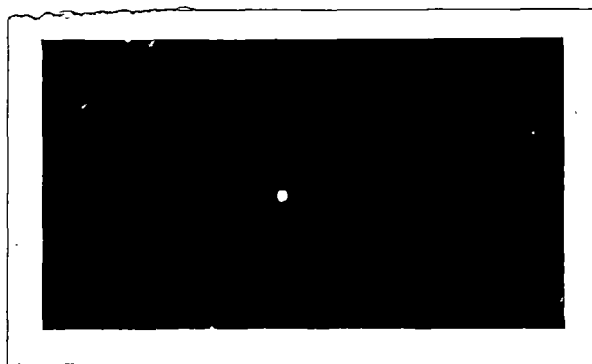


Plate 3b: X-ray diffraction photograph of the oriented sample in the nematic phase of CPPCC at 69°C.

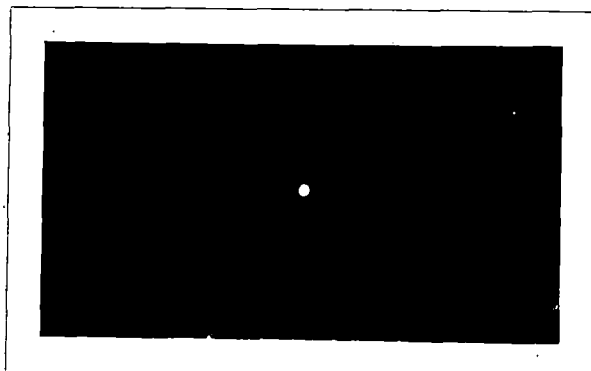


Plate 3c: X-ray diffraction photograph of the oriented sample in the nematic phase of CPBCC at 30.5°C.

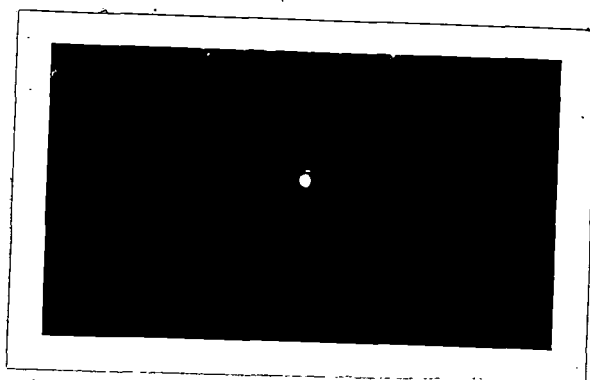


Plate 3d: X-ray diffraction photograph of the oriented sample in the nematic phase of CPBCC at 65°C.

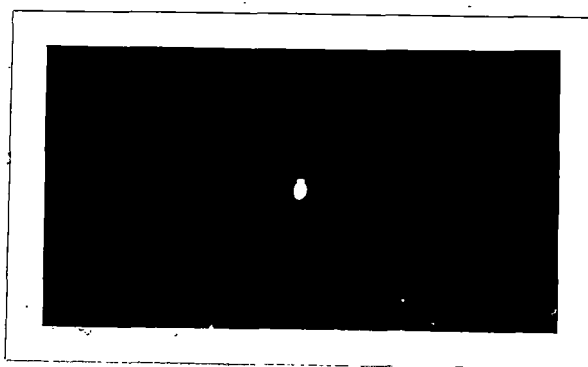


Plate 3e: X-ray diffraction photograph of the oriented sample in the nematic phase of BPPCC at 45°C.

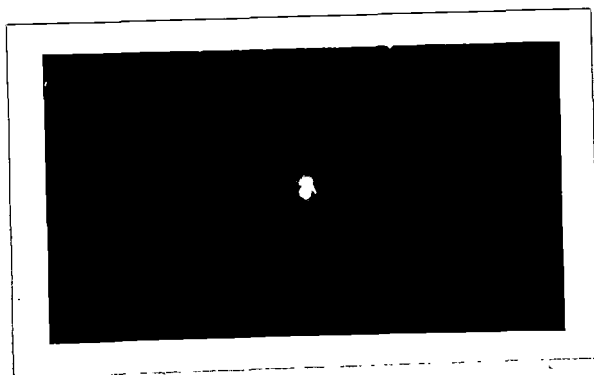


Plate 3f: X-ray diffraction photograph of the oriented sample in the nematic phase of BPPCC at 70°C.

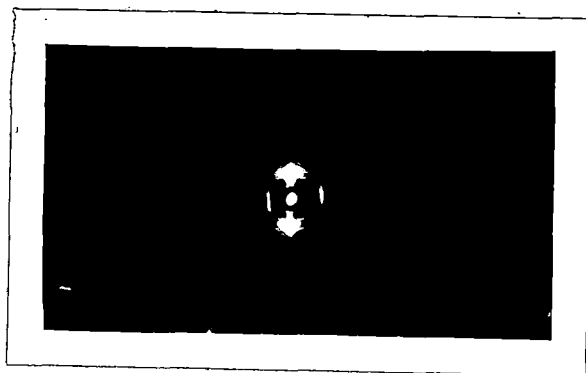


Plate 3g: X-ray diffraction photograph of the partially oriented sample in the smectic phase of PPPCC at 35°C.

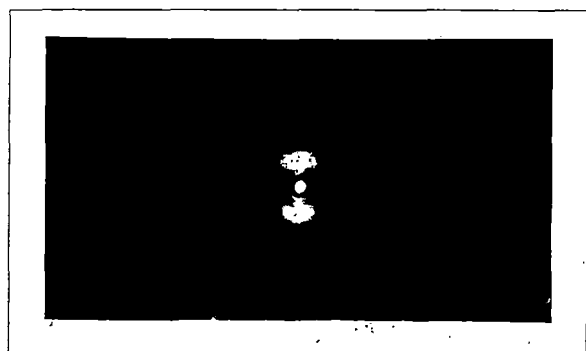


Plate 3h: X-ray diffraction photograph of the oriented sample in the nematic phase of PPPCC at 40°C.

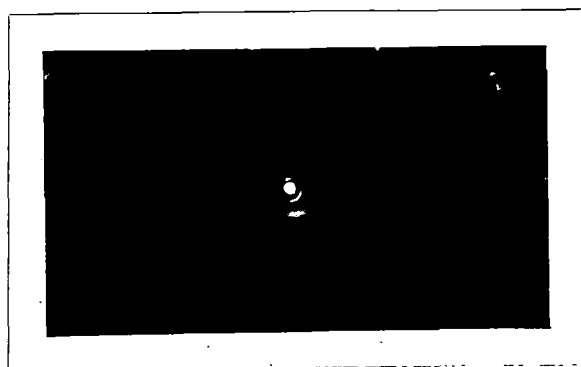


Plate 3i: X-ray diffraction photograph of the oriented sample in the nematic phase of PPPCC at 74.5°C.

not be aligned in the applied magnetic field of about 5 Kilogauss. Moreover, even in the nematic phase of this compound, strong smectic like inner spot were observed in the x-ray pattern upto 40 °C(Plate 3h). Hence, PPPCC has cybotactic nematic phase below 40 °C. Above 40°C the x-ray diffraction pattern is like normal nematic(Plate3i).

The experimental magnetic susceptibility values at different temperatures along the director for CPPCC, CPBCC, BPPCC and PPPCC are tabulated in Tables 3.37 to 3.40. The values of respective magnetic susceptibilities in the isotropic phases are also given in these Tables. The magnetic susceptibility anisotropies in the perfectly ordered state,  $\Delta\chi_0$ , have been determined by Haller's extrapolation (Chapter 2) procedure and are noted in the respective Table. The calculated magnetic susceptibility anisotropy ( $\Delta\chi$ ) and order parameter values are also shown in these tables. The temperature variation of magnetic anisotropy for all these four mesogens have been shown in Figures 3.10 to 3.13. In all these compounds  $\Delta\chi$  decreases monotonically with increasing temperature and shows a discontinuity at the nematic to isotropic phase transition.

The temperature variation of order parameter values obtained from refractive index, magnetic susceptibility and x-ray diffraction studies for CPPCC, CPBCC, BPPCC, and PPPCC are shown in Figures 3.14, 3.15, 3.16 and 3.17 respectively. The theoretical Maier-Saupe order parameter values are also shown in these figures. For all the mesogens the trend is similar. At temperatures much below the nematic to isotropic transition, the experimental order parameter values are somewhat greater than the Maier-Saupe calculated values. Near the transition temperature the values of order parameters obtained from refractive index and magnetic susceptibility studies decreases rapidly with increasing temperature, so that

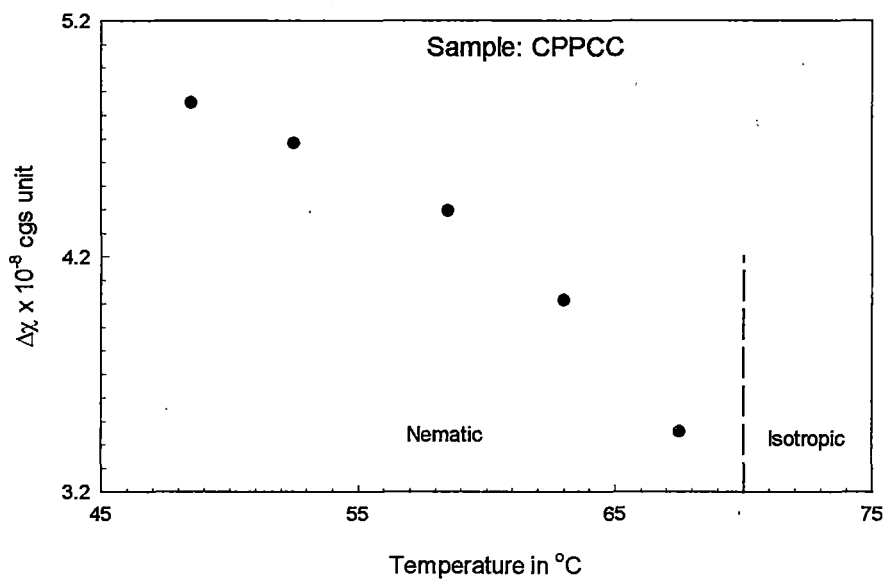


Figure 3.10. Temperature variation of the anisotropy of the diamagnetic susceptibility ( $\Delta\chi$ ).

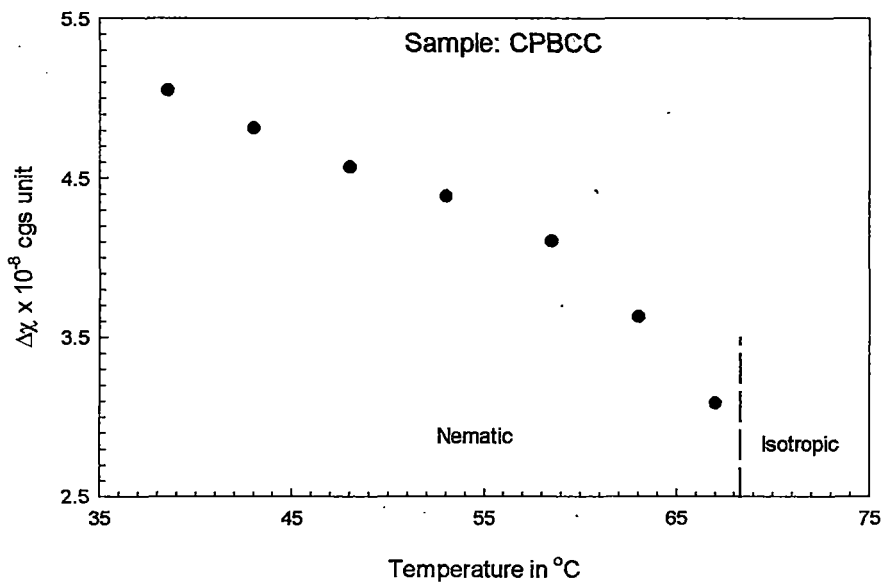


Figure 3.11. Temperature variation of the anisotropy of the diamagnetic susceptibility ( $\Delta\chi$ ).

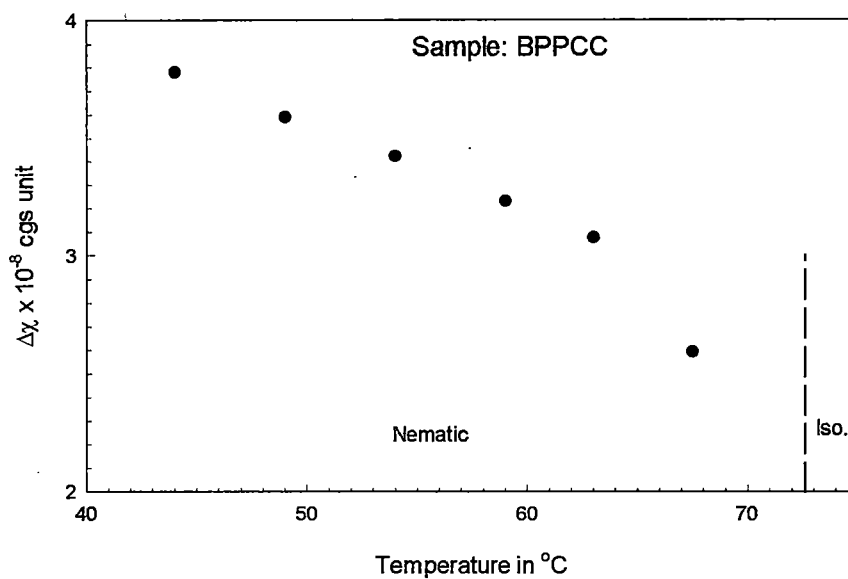


Figure 3.12. Temperature variation of the anisotropy of the diamagnetic susceptibility ( $\Delta\chi$ ).

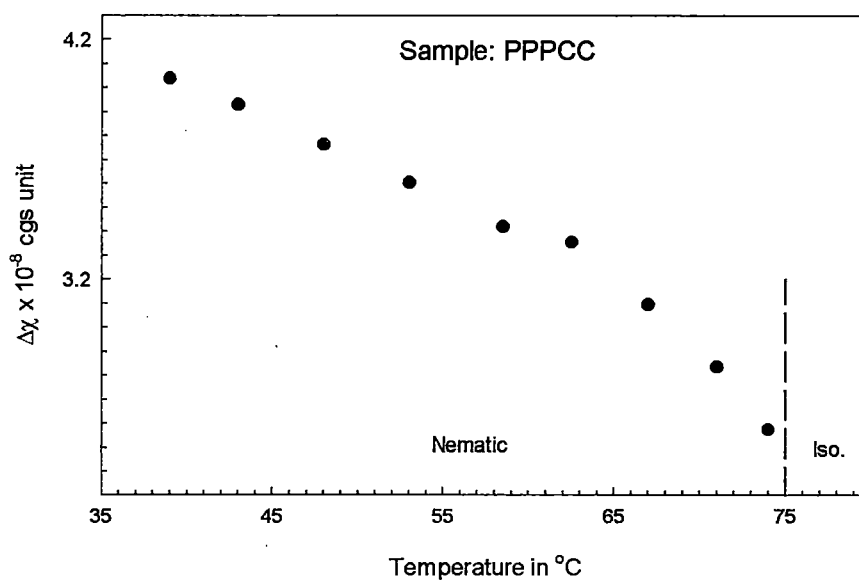


Figure 3.13. Temperature variation of the anisotropy of the diamagnetic susceptibility ( $\Delta\chi$ ).

these values are lower than the theoretical values. The order parameters from x-ray diffraction studies on the other hand follow the Maier-Saupe values closely near the clearing temperature. The rapid variation of  $\langle P_2 \rangle$  obtained from refractive index and magnetic susceptibility data near the N-I transition temperature has been observed by many workers [5-9]. This may be due to fluctuations of the director, which is more pronounced near the transition temperature. Moreover, in the present study all the four compounds have cyclohexane ring, which may vibrate more with the rise of temperature and thus lower the order parameter in addition to the lowering effect due to the aliphatic chain vibrations. However, x-ray studies do not show such rapid decrease of order parameter near the transition. This may be due to the fact that the x-ray diffraction pattern (outer arc) is due to the neighbouring molecules, hence we essentially measure the short range order parameter, which changes less rapidly near the transition temperature. In effect, we are measuring different order parameters depending upon the experimental method used and hence this discrepancy between different experimentally determined order parameter values.

The splay and bend elastic constants of CPPCC, CPBCC, BPPCC and PPPCC have been determined by observing Freedericksz transition in a magnetic field. The full experimental details of the experiment have been given in Chapter 2. The splay and bend elastic constant values together with the critical magnetic fields at different temperatures for the compound CPPCC are given in the Tables 3.41 and 3.42 respectively. The sample thicknesses and the interpolated values of the magnetic susceptibility anisotropy are also given in the Tables. Similarly  $K_{11}$  and  $K_{33}$  values of CPBCC are shown in Tables 3.43 and 3.44 respectively. The

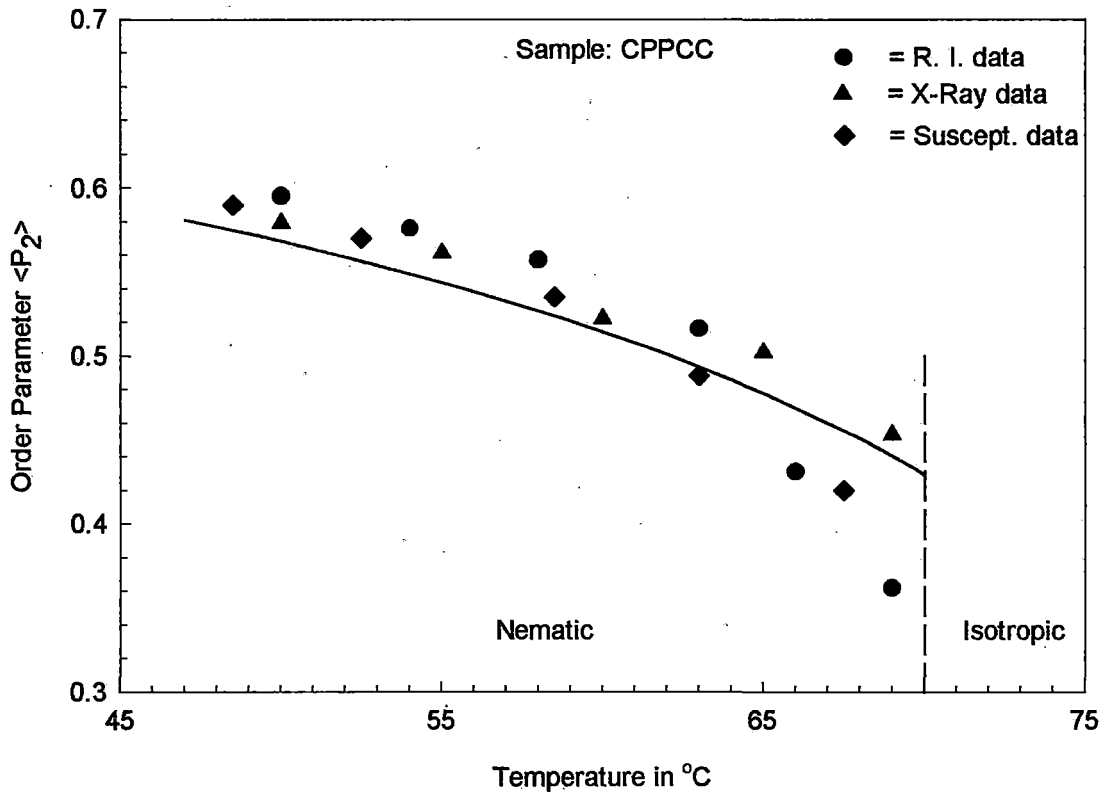


Figure 3.14. Temperature variation of Order Parameter  $\langle P_2 \rangle$ . Continuous curve corresponds to Maier-Saupe theoretical values.

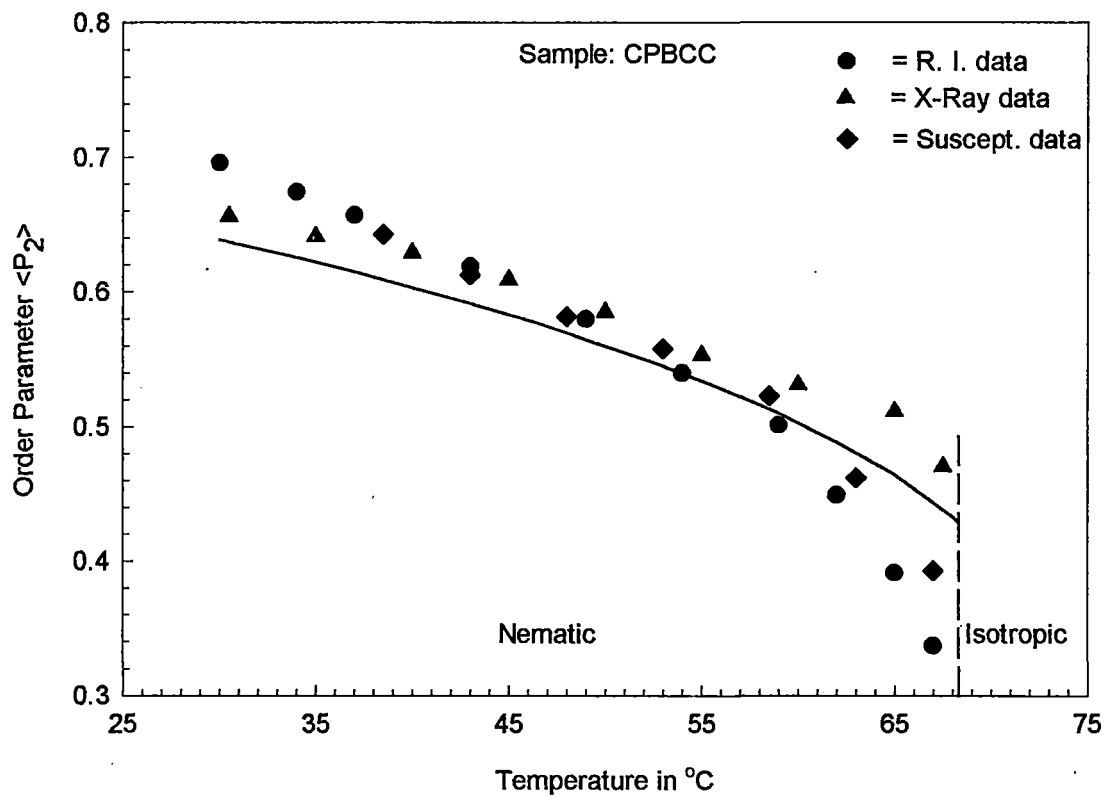


Figure 3.15. Temperature variation of Order Parameter  $\langle P_2 \rangle$ . Continuous curve corresponds to Maier-Saupe theoretical values.

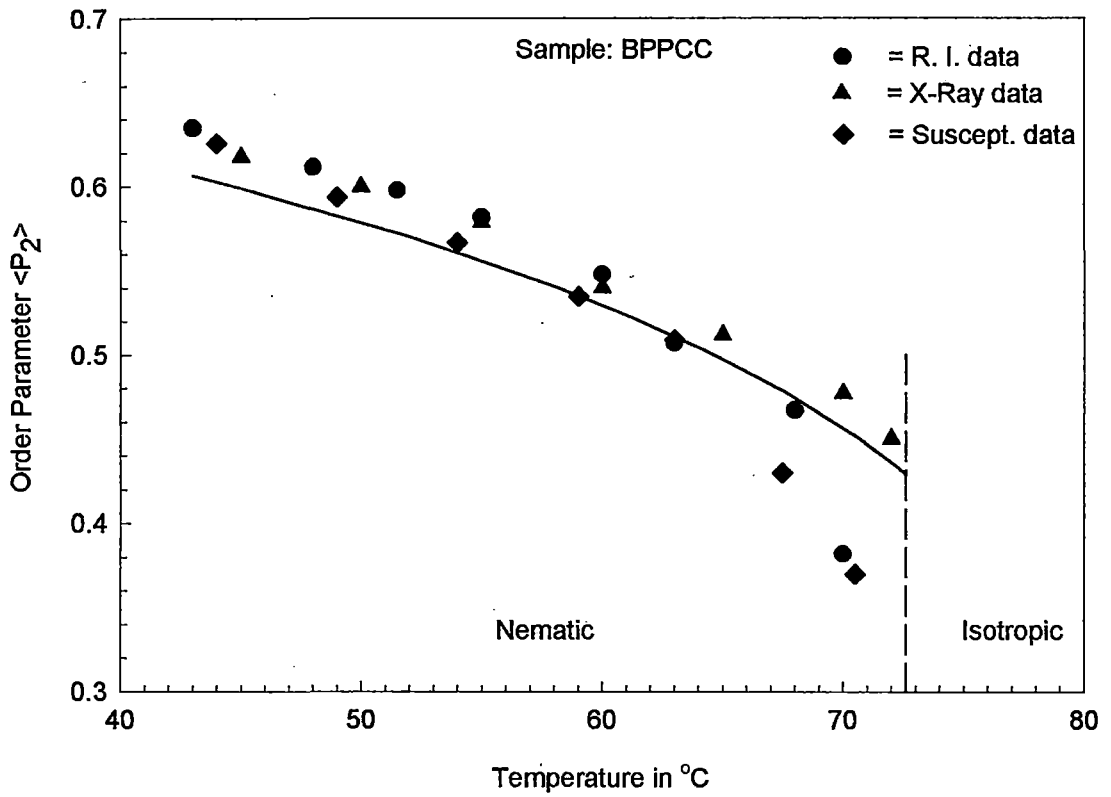


Figure 3.16. Temperature variation of Order Parameter  $\langle P_2 \rangle$ . Continuous curve corresponds to Maier-Saupe theoretical values.

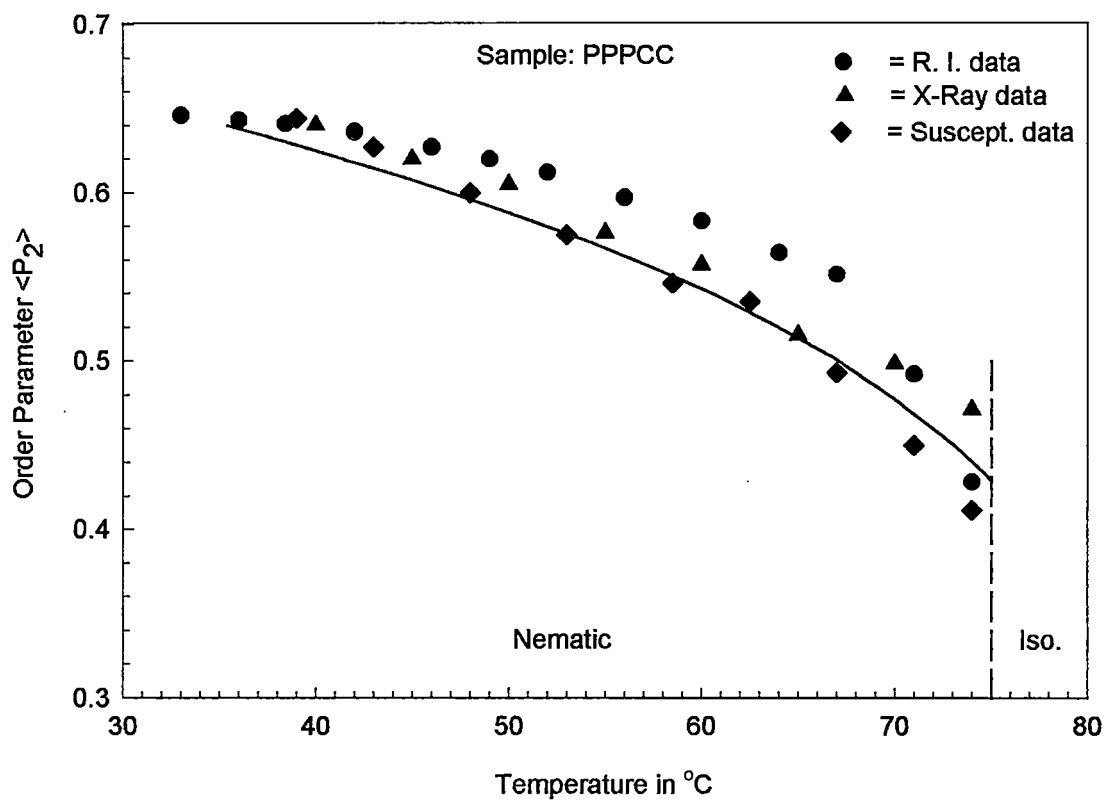


Figure 3.17. Temperature variation of Order Parameter  $\langle P_2 \rangle$ . Continuous curve corresponds to Maier-Saupe theoretical values.

splay and bend elastic constant values for BPPCC and PPPCC are tabulated in Tables 3.45 to 3.48. The ratios of bend to splay elastic constants ( $K_{33}/K_{11}$ ) at different relative temperatures for these four mesogens are given in Tables 3.49 and 3.50. The temperature variation of splay and bend elastic constants for CPPCC, CPBCC, BPPCC, and PPPCC are shown in Figures 3.26 to 3.29. Scharkowski et al [10] have given a figure showing the variation of  $K_{33}/K_{11}$  with reduced temperature for the two cyano compounds (CPPCC and CPBCC) studied by us. However, they have not given the values of  $K_{11}$  and  $K_{33}$  separately, so we cannot compare our splay and bend elastic constant values with their values directly. Our bend to splay ratios show similar temperature variations as observed by Scharkowski et al [10]. In both CPPCC and CPBCC the ratios are always greater than 1 and increases with decreasing temperatures. The ratios are somewhat larger for CPPCC than for CPBCC. However, our bend to splay elastic constant ratios are almost 15% smaller than those given by Scharkowski et al. We are unable to explain this discrepancy, since individual  $K_{11}$  and  $K_{33}$  values are not given by them. The other two mesogens (BPPCC and PPPCC) have the bend to splay ratios less than 1 at all temperatures. Schadt et al [11] have also reported that  $K_{33}/K_{11}$  is less than 1 for related compound 5CEPO3 in which the pentyloxy group in PPPCC has been replaced by propyloxy group. In BPPCC the  $K_{33}/K_{11}$  ratio increases slowly as the temperature decreases as in CPPCC and CPBCC. However, in PPPCC the bend to splay ratio decreases quite rapidly with decreasing temperatures. It may be mentioned that from the x-ray diffraction studies PPPCC shows cybotactic nematic phase. In the cybotactic nematic phase small groups of molecules show smectic like order. It has been pointed out by Bradshaw et al [12] that smectic like

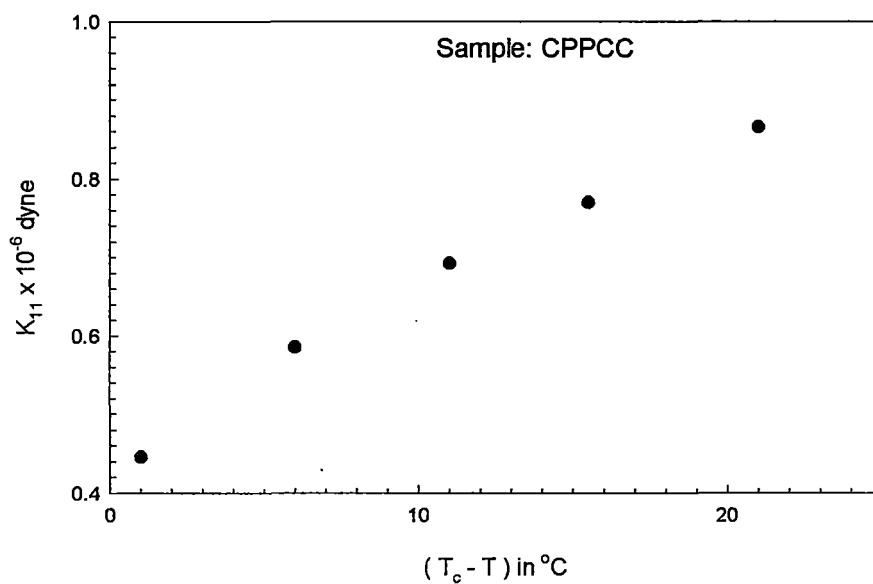


Figure 3.18. Splay elastic constant ( $K_{11}$ ) as a function of relative temperature ( $T_c - T$ ).

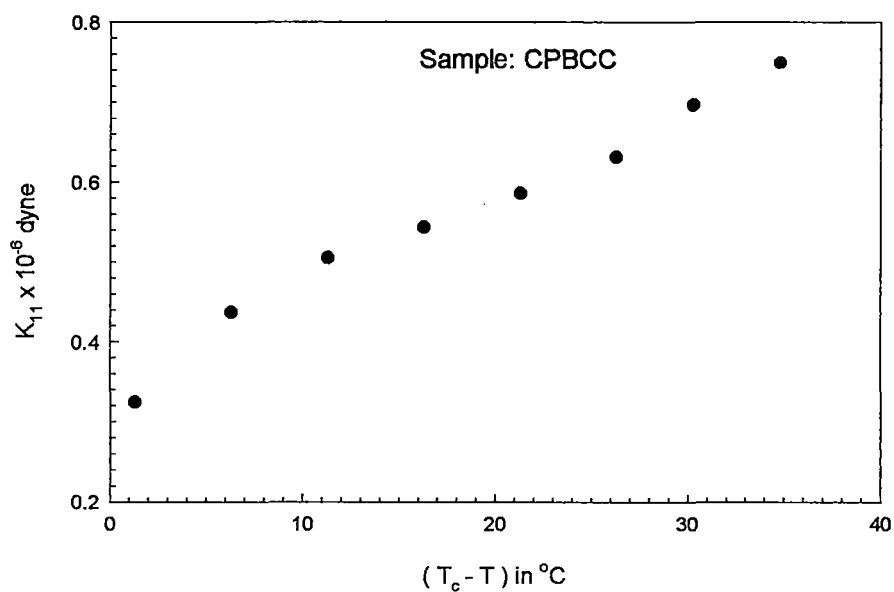


Figure 3.19. Splay elastic constant ( $K_{11}$ ) as a function of relative temperature ( $T_c - T$ ).

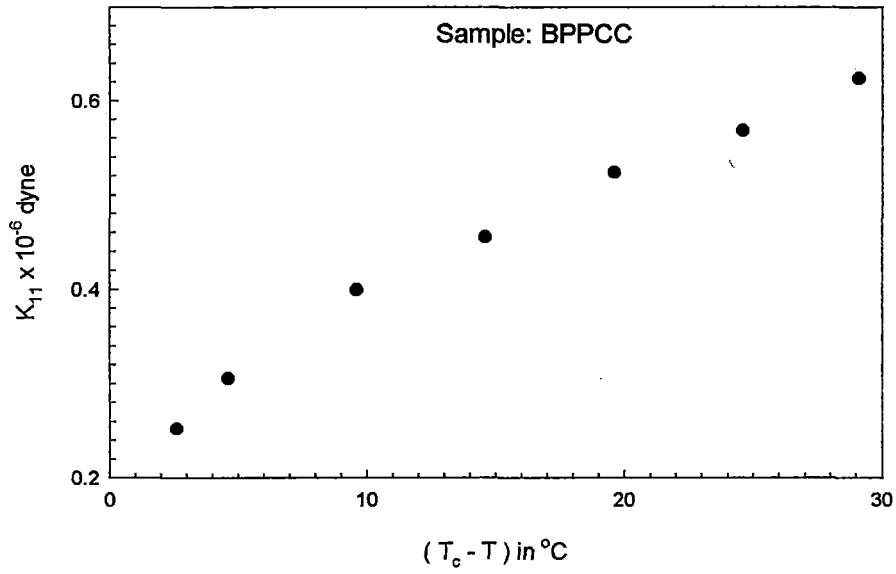


Figure 3.20. Splay elastic constant ( $K_{11}$ ) as a function of relative temperature ( $T_c - T$ ).

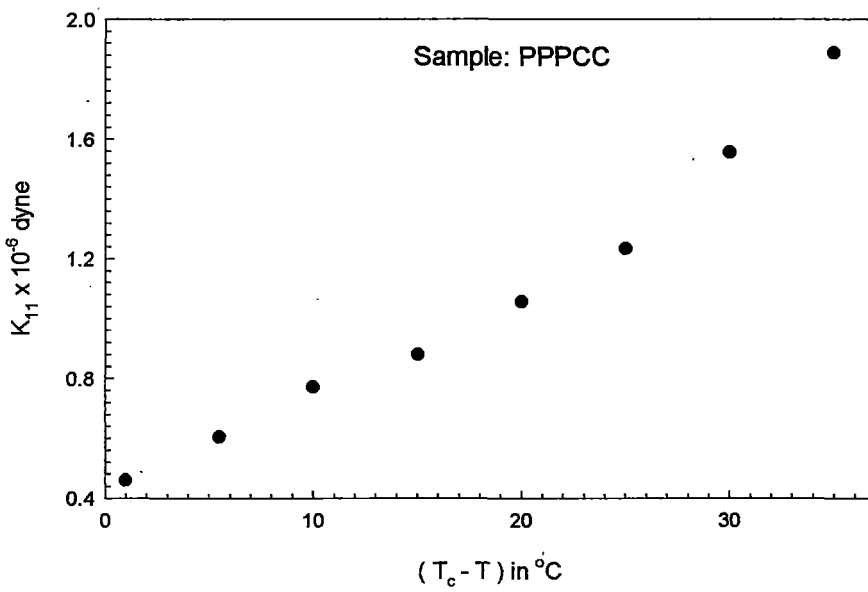


Figure 3.21. Splay elastic constant ( $K_{11}$ ) as a function of relative temperature ( $T_c - T$ ).

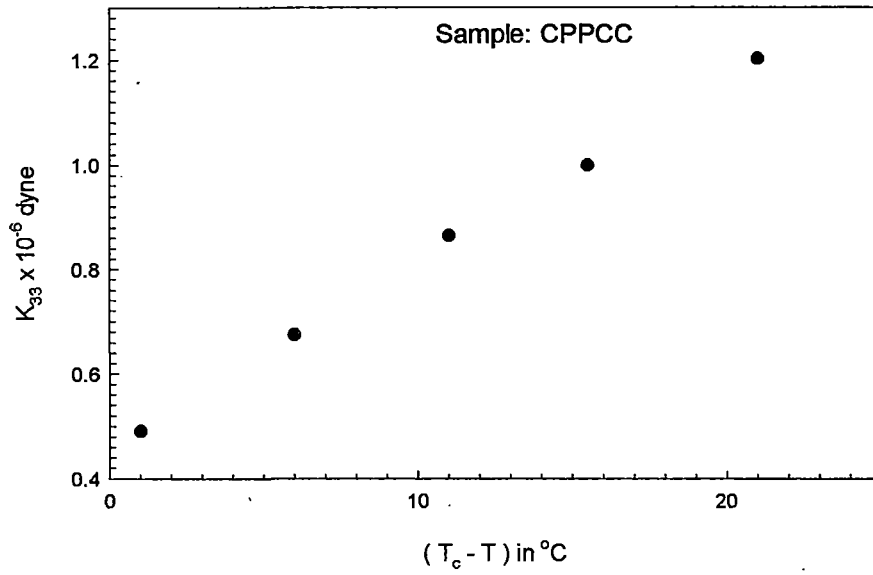


Figure 3.22. Bend elastic constant ( $K_{33}$ ) as a function of relative temperature ( $T_c - T$ ).

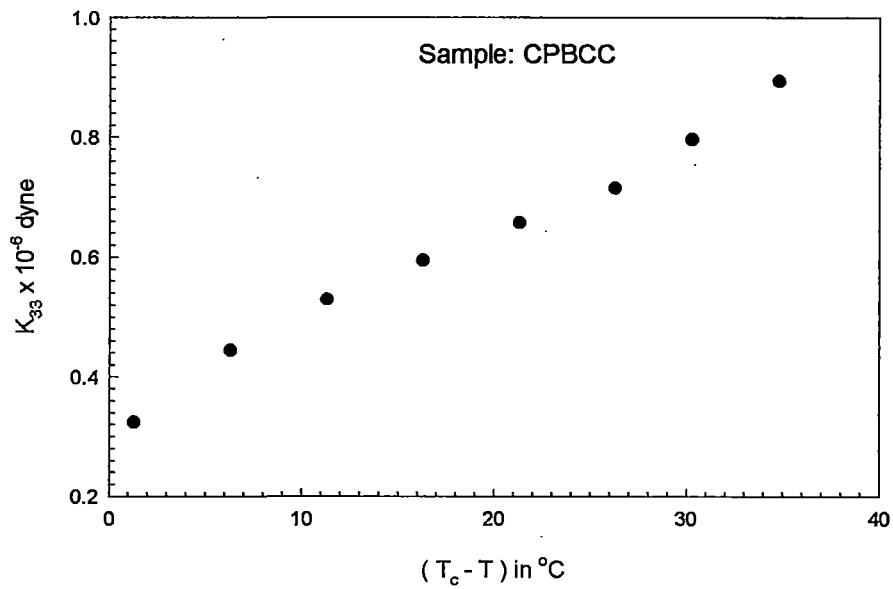


Figure 3.23. Bend elastic constant ( $K_{33}$ ) as a function of relative temperature ( $T_c - T$ ).

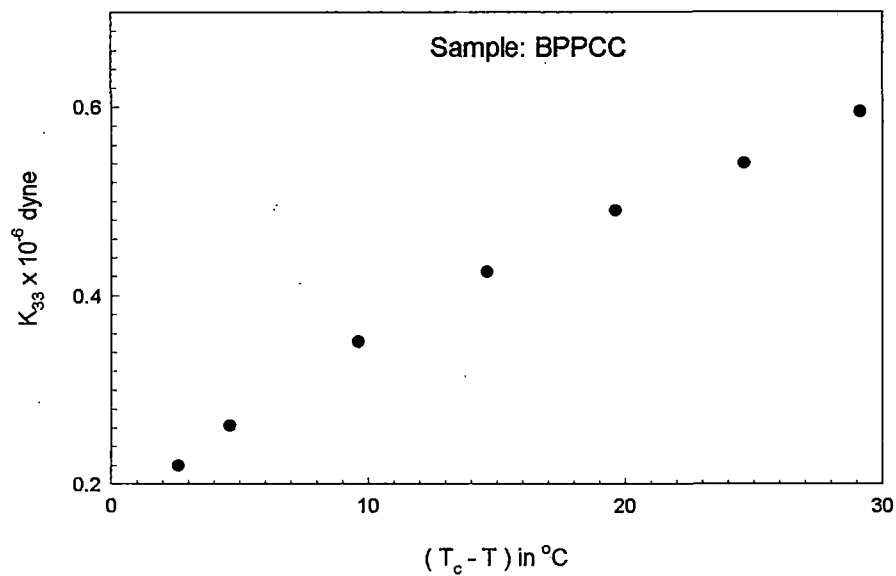


Figure 3.24. Bend elastic constant ( $K_{33}$ ) as a function of relative temperature ( $T_c - T$ ).

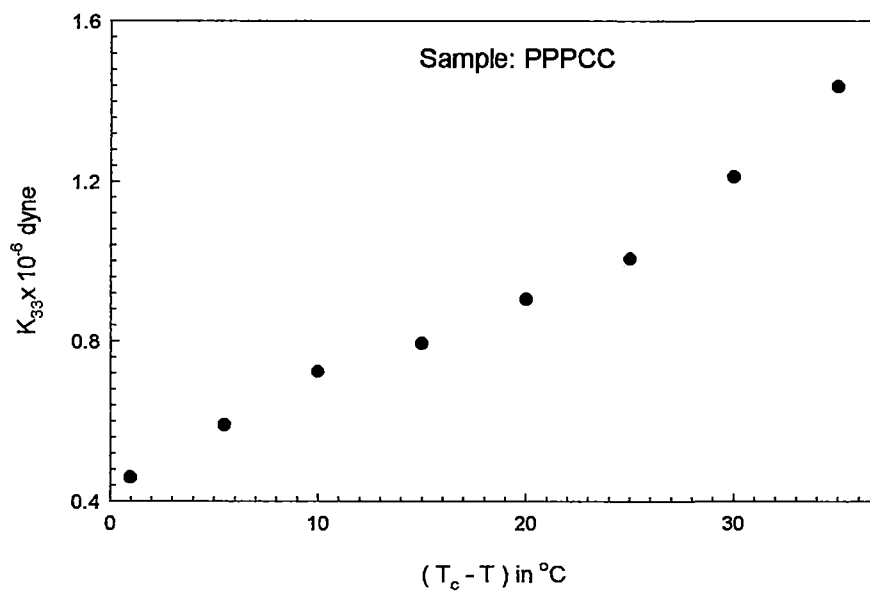


Figure 3.25. Bend elastic constant ( $K_{33}$ ) as a function of relative temperature ( $T_c - T$ ).

local ordering in nematogens increases  $K_{11}$  and thus lowers the value of  $K_{33}/K_{11}$ . The temperature variation of  $K_{11}$  in PPPCC indeed shows rapid change (Figure 3.21). Hence the decrease in the  $K_{33}/K_{11}$  ratio in PPPCC with decreasing temperature can safely be attributed to the presence of smectic like cybotactic groups.

According to Schadt et al [11], the  $K_{33}/K_{11}$  ratio in polar compounds are larger than non-polar compounds having related structure. Thus we find that polar CPPCC and CPBCC have  $K_{33}/K_{11}$  greater than 1, whereas in their related non-polar compounds BPPCC and PPPCC the same ratio is less than 1.

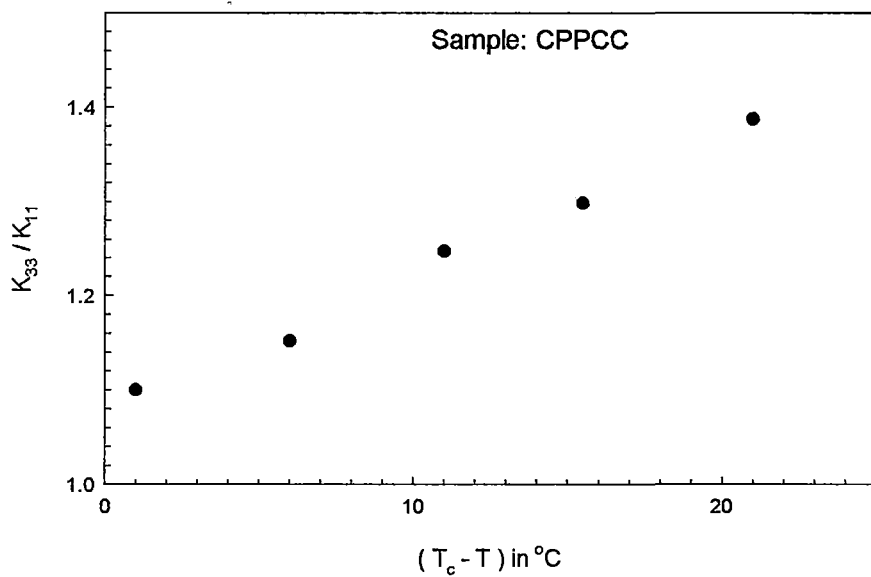


Figure 3.26. Bend to Splay elastic constant ratio ( $K_{33}/K_{11}$ ) as a function of relative temperature ( $T_c - T$ ).

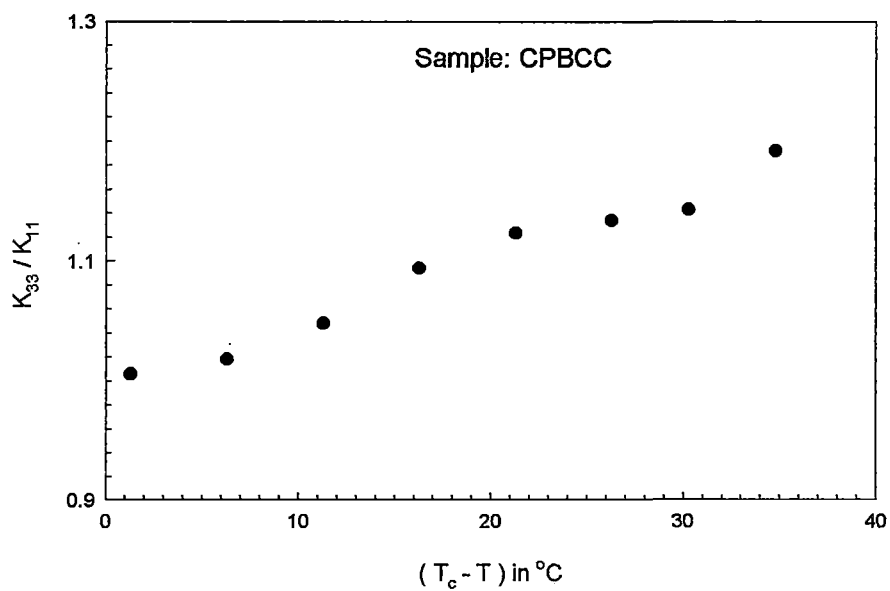


Figure 3.27. Bend to Splay elastic constant ratio ( $K_{33}/K_{11}$ ) as a function of relative temperature ( $T_c - T$ ).

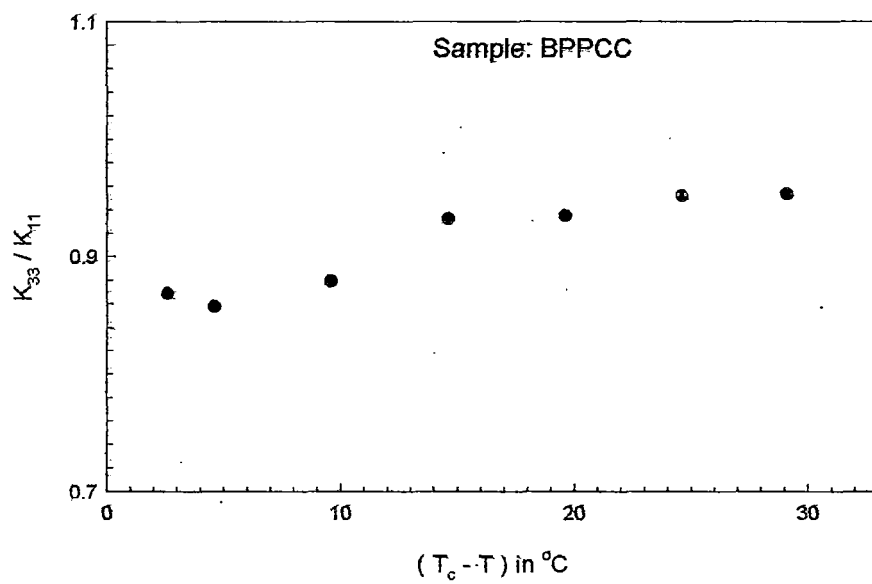


Figure 3.28. Bend to Splay elastic constant ratio ( $K_{33} / K_{11}$ ) as a function of relative temperature ( $T_c - T$ ).

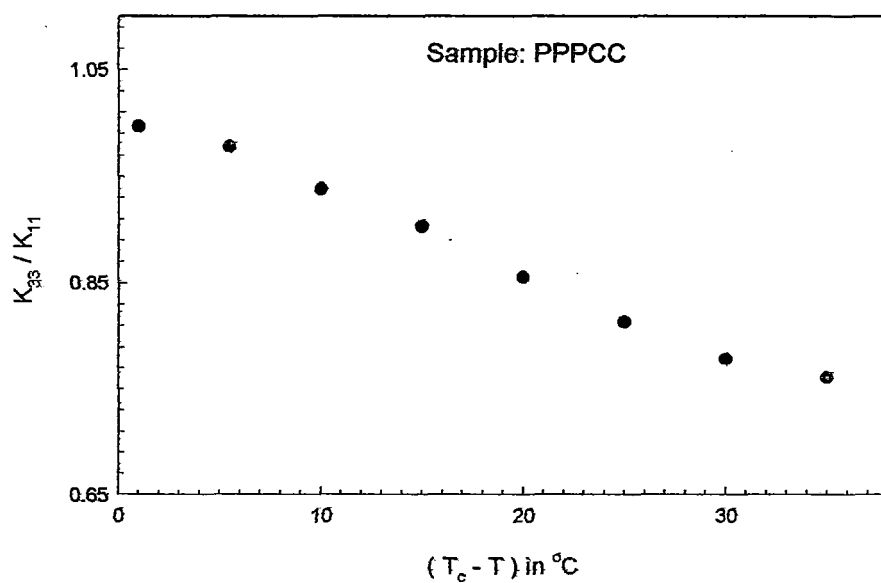


Figure 3.29. Bend to Splay elastic constant ratio ( $K_{33} / K_{11}$ ) as a function of relative temperature ( $T_c - T$ ).

**Table 3.1a**

**Density ( $\rho$ ) and refractive indices ( $n_o$ ,  $n_e$ ) at different temperatures of Sample CPPCC.**

Temp. in ° C	Density in gm/cc	$\lambda = 6907 \text{ \AA}$		$\lambda = 5780 \text{ \AA}$	
		$n_o$	$n_e$	$n_o$	$n_e$
50	1.068	1.464	1.564	1.471	1.571
54	1.066	1.464	1.561	1.471	1.568
58	1.063	1.464	1.557	1.471	1.564
63	1.057	1.464	1.550	1.471	1.557
66	1.053	1.471	1.543	1.479	1.550
69	1.049	1.475	1.536	1.482	1.543
71	1.044	1.493		1.500	

**Table 3.1b**

**Density ( $\rho$ ) and refractive indices ( $n_o$ ,  $n_e$ ) at different temperatures of Sample CPPCC.**

Temp. in ° C	Density in gm/cc	$\lambda = 5461 \text{ \AA}$		$\lambda = 4358 \text{ \AA}$	
		$n_o$	$n_e$	$n_o$	$n_e$
50	1.068	1.479	1.579	1.489	1.589
54	1.066	1.479	1.575	1.489	1.586
58	1.063	1.479	1.571	1.489	1.582
63	1.057	1.479	1.564	1.489	1.575
66	1.053	1.486	1.557	1.496	1.568
69	1.049	1.489	1.550	1.050	1.561
71	1.044	1.507		1.521	

**Table 3.2a**

**Density ( $\rho$ ) and refractive indices ( $n_o$ ,  $n_e$ ) at different temperatures of Sample CPBCC.**

Temp. in °C	Density in gm/cc	$\lambda = 6907 \text{ \AA}$		$\lambda = 5780 \text{ \AA}$	
		$n_o$	$n_e$	$n_o$	$n_e$
30	1.049	1.472	1.592	1.479	1.599
34	1.047	1.472	1.588	1.479	1.595
37	1.045	1.472	1.585	1.479	1.592
43	1.041	1.472	1.577	1.479	1.585
49	1.035	1.472	1.570	1.479	1.577
54	1.032	1.472	1.563	1.479	1.570
59	1.026	1.472	1.556	1.479	1.563
62	1.023	1.474	1.549	1.481	1.556
65	1.019	1.477	1.542	1.484	1.549
67	1.016	1.479	1.535	1.486	1.542
69	1.013		1.493		1.500

**Table 3.2b**

**Density ( $\rho$ ) and refractive indices ( $n_o$ ,  $n_e$ ) at different temperatures of Sample CPBCC.**

Temp. in °C	Density in gm/cc	$\lambda = 5461 \text{ \AA}$		$\lambda = 4358 \text{ \AA}$	
		$n_o$	$n_e$	$n_o$	$n_e$
30	1.049	1.486	1.606	1.496	1.616
34	1.047	1.486	1.602	1.496	1.612
37	1.045	1.486	1.599	1.496	1.609
43	1.041	1.486	1.592	1.496	1.602
49	1.035	1.486	1.585	1.496	1.595
54	1.032	1.486	1.577	1.496	1.588
59	1.026	1.486	1.570	1.496	1.581
62	1.023	1.488	1.563	1.498	1.574
65	1.019	1.491	1.556	1.501	1.567
67	1.016	1.493	1.549	1.504	1.560
69	1.013	1.507		1.518	

**Table 3.3a**

**Density ( $\rho$ ) and refractive indices ( $n_o$ ,  $n_e$ ) at different temperatures of Sample BPPCC.**

Temp. in °C	Density in gm/cc	$\lambda = 6907 \text{ \AA}$		$\lambda = 5780 \text{ \AA}$	
		$n_o$	$n_e$	$n_o$	$n_e$
43	0.993	1.452	1.556	1.459	1.563
48	0.989	1.451	1.551	1.458	1.558
51.5	0.985	1.451	1.548	1.457	1.554
55	0.983	1.450	1.544	1.457	1.551
60	0.979	1.449	1.537	1.456	1.544
63	0.976	1.449	1.531	1.456	1.537
68	0.972	1.449	1.524	1.456	1.531
70	0.970	1.456	1.517	1.463	1.524
73	0.964	1.476		1.483	

**Table 3.3b**

**Density ( $\rho$ ) and refractive indices ( $n_o$ ,  $n_e$ ) at different temperatures of Sample BPPCC.**

Temp. in ° C	Density in gm/cc	$\lambda = 5461 \text{ \AA}$		$\lambda = 4358 \text{ \AA}$	
		$n_o$	$n_e$	$n_o$	$n_e$
43	0.993	1.466	1.570	1.476	1.580
48	0.989	1.465	1.565	1.475	1.575
51.5	0.985	1.464	1.561	1.474	1.571
55	0.983	1.464	1.558	1.474	1.568
60	0.979	1.463	1.551	1.473	1.561
63	0.976	1.463	1.544	1.473	1.554
68	0.972	1.463	1.537	1.473	1.548
70	0.970	1.469	1.531	1.480	1.541
73	0.964	1.490		1.500	

**Table 3.4a**

**Density ( $\rho$ ) and refractive indices ( $n_o$ ,  $n_e$ ) at different temperatures of Sample PPPCC.**

Temp. in °C	Density in gm/cc	$\lambda = 6907 \text{ \AA}$		$\lambda = 5780 \text{ \AA}$	
		$n_o$	$n_e$	$n_o$	$n_e$
33	0.981	1.469	1.560	1.476	1.567
36	0.977	1.469	1.559	1.476	1.566
38.4	0.976	1.469	1.559	1.476	1.565
42	0.973	1.469	1.558	1.476	1.565
46	0.970	1.468	1.555	1.475	1.562
49	0.967	1.467	1.553	1.474	1.560
52	0.965	1.467	1.551	1.473	1.558
56	0.962	1.466	1.548	1.472	1.554
60	0.958	1.464	1.544	1.471	1.551
64	0.955	1.463	1.540	1.470	1.547
67	0.952	1.463	1.537	1.469	1.544
71	0.948	1.464	1.531	1.471	1.537
74	0.944	1.466	1.524	1.473	1.531
76	0.941	1.483		1.490	

**Table 3.4b**

**Density ( $\rho$ ) and refractive indices ( $n_o$ ,  $n_e$ ) at different temperatures of Sample PPPCC.**

Temp. in ° C	Density in gm/cc	$\lambda = 5461 \text{ \AA}$		$\lambda = 4358 \text{ \AA}$	
		$n_o$	$n_e$	$n_o$	$n_e$
33	0.981	1.483	1.573	1.493	1.584
36	0.977	1.483	1.573	1.493	1.583
38.4	0.976	1.483	1.572	1.493	1.582
42	0.973	1.483	1.571	1.493	1.582
46	0.970	1.482	1.569	1.492	1.579
49	0.967	1.481	1.567	1.491	1.577
52	0.965	1.480	1.565	1.490	1.575
56	0.962	1.479	1.561	1.489	1.571
60	0.958	1.478	1.558	1.488	1.568
64	0.955	1.477	1.554	1.487	1.564
67	0.952	1.476	1.551	1.486	1.561
71	0.948	1.478	1.544	1.488	1.554
74	0.944	1.480	1.537	1.490	1.548
76	0.941	1.497		1.507	

**Table 3.5**

**Polarisability ( $\alpha_o, \alpha_e$ ) at different temperatures of sample CPPCC  
by Vuks method.**

Temp. in °C	$\lambda = 6907 \text{ \AA}$		$\lambda = 5780 \text{ \AA}$		$\lambda = 5461 \text{ \AA}$		$\lambda = 4358 \text{ \AA}$	
	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$
50	27.11	34.28	27.46	34.64	27.82	35.00	28.35	35.51
54	27.19	34.11	27.54	34.48	27.90	34.83	28.43	35.36
58	27.30	33.99	27.65	34.34	28.01	34.70	28.55	35.23
63	27.50	33.70	27.85	34.07	28.22	34.42	28.75	34.96
66	28.04	33.23	28.41	33.59	28.77	33.95	29.31	34.48
69	28.40	32.82	28.77	33.19	29.13	33.55	29.88	34.03

$\alpha_o$  &  $\alpha_e$  are in  $10^{-24} \text{ cm}^3$  unit.

**Table 3.6**

**Polarisability ( $\alpha_o, \alpha_e$ ) at different temperatures of sample CPBCC  
by Vuks method.**

Temp. in °C	$\lambda = 6907 \text{ \AA}$		$\lambda = 5780 \text{ \AA}$		$\lambda = 5461 \text{ \AA}$		$\lambda = 4358 \text{ \AA}$	
	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$
30	29.29	38.50	29.66	38.88	30.04	39.23	30.59	39.79
34	29.38	38.29	29.75	38.66	30.13	39.04	30.68	39.59
37	29.46	38.16	29.83	38.53	30.21	38.90	30.76	39.45
43	29.63	37.81	30.00	38.19	30.38	38.56	30.94	39.12
49	29.82	37.50	30.20	37.87	30.58	38.25	31.15	38.81
54	29.99	37.13	30.37	37.51	30.75	37.89	31.32	38.45
59	30.21	36.84	30.60	37.22	30.98	37.61	31.55	38.17
62	30.46	36.41	30.85	36.79	31.24	37.18	31.81	37.74
65	30.80	35.97	31.18	36.36	31.57	36.74	32.14	37.32
67	31.09	35.54	31.48	35.92	31.86	36.31	32.45	36.89

$\alpha_o$  &  $\alpha_e$  are in  $10^{-24} \text{ cm}^3$  unit.

**Table 3.7**

**Polarisability ( $\alpha_o, \alpha_e$ ) at different temperatures of sample BPPCC  
by Vuks method.**

Temp. in °C	$\lambda = 6907 \text{ \AA}$		$\lambda = 5780 \text{ \AA}$		$\lambda = 5461 \text{ \AA}$		$\lambda = 4358 \text{ \AA}$	
	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$
43	33.43	42.83	33.87	43.27	34.29	43.69	34.94	44.34
48	33.52	42.60	33.97	43.02	34.39	43.46	35.04	44.09
51.5	33.62	42.47	34.06	42.91	34.49	43.34	35.15	43.98
55	33.69	42.31	34.13	42.75	34.56	43.18	35.22	43.83
60	33.80	41.92	34.25	42.36	34.69	42.81	35.35	43.46
63	33.97	41.48	34.42	41.93	34.86	42.37	35.53	43.02
68	34.18	41.09	34.62	41.53	35.07	41.98	35.74	42.64
70	34.80	40.47	35.25	40.91	35.70	41.35	36.36	42.01

$\alpha_o$  &  $\alpha_e$  are in  $10^{-24} \text{ cm}^3$  unit.

**Table 3.8**

**Polarisability ( $\alpha_o, \alpha_e$ ) at different temperatures of sample PPPCC  
by Vuks method.**

Temp. in °C	$\lambda = 6907 \text{ \AA}$		$\lambda = 5780 \text{ \AA}$		$\lambda = 5461 \text{ \AA}$		$\lambda = 4358 \text{ \AA}$	
	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$
33	39.68	4906	4017	49.54	40.66	50.04	41.39	50.76
36	39.82	49.17	40.32	49.65	40.81	50.15	41.54	50.87
38.4	39.89	49.19	40.39	49.68	40.88	50.17	41.61	50.91
42	40.00	49.23	40.49	49.73	40.99	50.22	41.72	50.96
46	40.07	49.17	40.57	49.67	41.07	50.16	41.81	50.90
49	40.14	49.14	40.64	49.63	41.14	50.13	41.88	50.87
52	40.19	49.08	40.69	49.57	41.19	50.07	41.93	50.81
56	40.24	48.91	40.75	49.41	41.25	49.91	42.00	50.65
60	40.34	48.79	40.85	49.31	41.35	49.80	42.10	50.56
64	40.42	48.61	40.93	49.11	41.44	49.62	42.19	50.37
67	40.53	48.53	41.05	49.03	41.55	49.55	42.31	50.30
71	40.87	48.00	41.39	48.51	41.90	49.02	42.66	49.78
74	41.28	47.49	41.80	48.00	42.31	48.53	43.08	49.29

$\alpha_o$  &  $\alpha_e$  are in  $10^{-24} \text{ cm}^3$  unit.

**Table 3.9**

**Polarisability ( $\alpha_o, \alpha_e$ ) at different temperatures of sample CPPCC  
by Neugebauer method.**

Temp. in °C	$\lambda = 6907 \text{ \AA}$		$\lambda = 5780 \text{ \AA}$		$\lambda = 5461 \text{ \AA}$		$\lambda = 4358 \text{ \AA}$	
	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$
50	27.50	33.50	27.85	33.85	28.22	34.19	28.76	34.70
54	27.57	33.36	27.92	33.72	28.29	34.06	28.83	34.57
58	27.66	33.26	28.02	33.61	28.38	33.96	28.92	34.47
63	27.83	33.03	28.19	33.39	28.56	33.74	29.10	34.26
66	28.32	32.67	28.69	33.02	29.05	33.38	29.60	33.90
69	28.64	32.35	29.01	32.71	29.38	33.06	30.11	33.57

$\alpha_o$  &  $\alpha_e$  are in  $10^{-24} \text{ cm}^3$  unit.

**Table 3.10**

**Polarisability ( $\alpha_o, \alpha_e$ ) at different temperatures of sample CPBCC  
by Neugebauer method.**

Temp. in ° C	$\lambda = 6907 \text{ \AA}$		$\lambda = 5780 \text{ \AA}$		$\lambda = 5461 \text{ \AA}$		$\lambda = 4358 \text{ \AA}$	
	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$
30	29.80	37.47	30.18	37.83	30.57	38.18	31.13	38.72
34	29.88	37.30	30.25	37.66	30.64	38.02	31.20	38.55
37	29.94	37.19	30.32	37.55	30.70	37.91	31.27	38.44
43	30.08	36.90	30.46	37.27	30.85	37.63	31.41	38.17
49	30.25	36.65	30.63	37.02	31.02	37.39	31.59	37.93
54	30.38	36.35	30.76	36.72	31.15	37.09	31.72	37.63
59	30.57	36.11	30.96	36.49	31.35	36.87	31.93	37.42
62	30.79	35.76	31.18	36.14	31.57	36.52	32.14	37.07
65	31.08	35.41	31.47	35.79	31.85	36.17	32.44	36.74
67	31.33	35.06	31.72	35.43	32.11	35.82	32.70	36.39

$\alpha_o$  &  $\alpha_e$  are in  $10^{-24} \text{ cm}^3$  unit.

**Table 3.11**

**Polarisability ( $\alpha_o, \alpha_e$ ) at different temperatures of sample BPPCC  
by Neugebauer method.**

Temp. in °C	$\lambda = 6907 \text{ \AA}$		$\lambda = 5780 \text{ \AA}$		$\lambda = 5461 \text{ \AA}$		$\lambda = 4358 \text{ \AA}$	
	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$
43	33.93	41.83	34.37	42.25	34.81	42.66	35.46	43.29
48	34.01	41.63	34.45	42.05	34.89	42.47	35.54	43.09
51.5	34.09	41.53	34.53	41.96	34.97	42.39	35.63	43.01
55	34.14	41.40	34.59	41.83	35.03	42.25	35.70	42.88
60	34.23	41.07	34.68	41.50	35.12	41.94	35.79	42.57
63	34.36	40.70	34.81	41.14	35.26	41.57	35.93	42.21
68	34.53	40.37	34.98	40.81	35.43	41.24	36.11	41.90
70	35.10	39.88	35.55	40.32	36.00	40.75	36.67	41.40

$\alpha_o$  &  $\alpha_e$  are in  $10^{-24} \text{ cm}^3$  unit.

**Table 3.12**

**Polarisability ( $\alpha_o, \alpha_e$ ) at different temperatures of sample PPPCC  
by Neugebauer method.**

Temp. in °C	$\lambda = 6907 \text{ \AA}$		$\lambda = 5780 \text{ \AA}$		$\lambda = 5461 \text{ \AA}$		$\lambda = 4358 \text{ \AA}$	
	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$	$\alpha_o$	$\alpha_e$
33	40.19	48.04	40.69	48.51	41.18	48.99	41.92	49.70
36	40.33	48.15	40.83	48.62	41.33	49.10	42.07	49.81
38.4	40.40	48.18	40.90	48.66	41.40	49.13	42.14	49.85
42	40.50	48.23	41.00	48.71	41.50	49.19	42.25	49.91
46	40.57	48.19	41.07	48.67	41.57	49.15	42.32	49.87
49	40.63	48.17	41.13	48.65	41.64	49.14	42.39	49.86
52	40.67	48.12	41.17	48.60	41.68	49.09	42.43	49.81
56	40.71	47.98	41.22	48.47	41.73	48.96	42.48	49.68
60	40.79	47.89	41.30	48.39	41.82	48.87	42.58	49.61
64	40.86	47.74	41.37	48.23	41.88	48.73	42.65	49.46
67	40.96	47.68	41.47	48.17	41.99	48.68	42.76	49.42
71	41.25	47.25	41.77	47.75	42.28	48.25	43.05	49.00
74	41.61	46.83	42.13	47.34	42.65	47.85	43.43	48.60

$\alpha_o$  &  $\alpha_e$  are in  $10^{-24} \text{ cm}^3$  unit.

**Table 3.13**

**Order parameter  $\langle P_2 \rangle$  of sample CPPCC at different temperatures by Vuks method.**

$$(\alpha_{\parallel} - \alpha_{\perp}) = 12.02 \text{ in } 10^{-24} \text{ cm}^3 \text{ unit.}$$

Temp. in °C	$\lambda = 6907 \text{ \AA}$	$\lambda = 5780 \text{ \AA}$	$\lambda = 5461 \text{ \AA}$	$\lambda = 4358 \text{ \AA}$	Average
	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$
50	0.596	0.591	0.597	0.596	.595
54	0.578	0.576	0.576	0.576	0.576
58	0.557	0.557	0.557	0.556	0.557
63	0.516	0.517	0.516	0.517	0.516
66	0.432	0.431	0.431	0.430	0.431
69	0.368	0.367	0.367	0.345	0.362

**Table 3.14**

**Order parameter  $\langle P_2 \rangle$  of sample CPBCC at different temperatures by Vuks method.**

$$(\alpha_{\parallel} - \alpha_{\perp}) = 13.22 \text{ in } 10^{-24} \text{ cm}^3 \text{ unit.}$$

Temp. in °C	$\lambda = 6907 \text{ \AA}$	$\lambda = 5780 \text{ \AA}$	$\lambda = 5461 \text{ \AA}$	$\lambda = 4358 \text{ \AA}$	Average
	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$
30	0.697	0.697	0.695	0.696	0.696
34	0.675	0.674	0.674	0.673	0.674
37	0.658	0.658	0.657	0.657	0.657
43	0.619	0.619	0.618	0.619	0.619
49	0.580	0.580	0.580	0.579	0.580
54	0.540	0.541	0.540	0.539	0.540
59	0.501	0.501	0.500	0.501	0.501
62	0.449	0.449	0.450	0.449	0.449
65	0.391	0.391	0.391	0.392	0.391
67	0.337	0.336	0.337	0.336	0.337

**Table3.15**

**Order parameter  $\langle P_2 \rangle$  of sample BPPCC at different temperatures by Vuks method.**

$$(\alpha_{\parallel} - \alpha_{\perp}) = 14.80 \text{ in } 10^{-24} \text{ cm}^3 \text{ unit.}$$

Temp. in °C	$\lambda = 6907 \text{ \AA}$	$\lambda = 5780 \text{ \AA}$	$\lambda = 5461 \text{ \AA}$	$\lambda = 4358 \text{ \AA}$	Average
	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$
43	0.635	0.635	0.635	0.635	0.635
48	0.613	0.611	0.613	0.611	0.612
51.5	0.598	0.598	0.598	0.597	0.598
55	0.582	0.583	0.582	0.581	0.582
60	0.549	0.547	0.549	0.548	0.548
63	0.507	0.507	0.507	0.507	0.507
68	0.467	0.467	0.467	0.467	0.467
70	0.383	0.380	0.382	0.382	0.382

**Table 3.16**

**Order parameter  $\langle P_2 \rangle$  of sample PPPCC at different temperatures by Vuks method.**

$$(\alpha_{\parallel} - \alpha_{\perp}) = 14.50 \text{ in } 10^{-24} \text{ cm}^3 \text{ unit.}$$

Temp. in °C	$\lambda = 6907 \text{ \AA}$	$\lambda = 5780 \text{ \AA}$	$\lambda = 5461 \text{ \AA}$	$\lambda = 4358 \text{ \AA}$	Average
	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$
33	0.647	0.646	0.647	0.646	0.646
36	0.644	0.643	0.644	0.643	0.643
38.4	0.641	0.641	0.641	0.641	0.641
42	0.637	0.636	0.636	0.637	0.636
46	0.628	0.627	0.627	0.627	0.627
49	0.621	0.620	0.620	0.620	0.620
52	0.613	0.612	0.613	0.612	0.612
56	0.597	0.597	0.597	0.597	0.597
60	0.583	0.583	0.583	0.583	0.583
64	0.565	0.564	0.565	0.564	0.564
67	0.552	0.550	0.551	0.551	0.551
71	0.492	0.492	0.492	0.491	0.492
74	0.428	0.428	0.429	0.428	0.428

**Table3.17**

**Order parameter  $\langle P_2 \rangle$  of sample CPPCC at different temperatures by Neugebauer method.**

$$(\alpha_{\parallel} - \alpha_{\perp}) = 10.08 \text{ in } 10^{-24} \text{ cm}^3 \text{ unit.}$$

Temp. in °C	$\lambda = 6907 \text{ \AA}$	$\lambda = 5780 \text{ \AA}$	$\lambda = 5461 \text{ \AA}$	$\lambda = 4358 \text{ \AA}$	Average
	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$
50	0.595	0.594	0.593	0.590	0.593
54	0.575	0.574	0.573	0.570	0.573
58	0.556	0.555	0.554	0.551	0.554
63	0.516	0.516	0.514	0.512	0.514
66	0.431	0.430	0.430	0.427	0.429
69	0.367	0.366	0.365	0.342	0.360

**Table 3.18**

**Order parameter  $\langle P_2 \rangle$  of sample CPBCC at different temperatures by Neugebauer method.**

$$(\alpha_{\parallel} - \alpha_{\perp}) = 11.04 \text{ in } 10^{-24} \text{ cm}^3 \text{ unit.}$$

Temp. in °C	$\lambda = 6907 \text{ \AA}$	$\lambda = 5780 \text{ \AA}$	$\lambda = 5461 \text{ \AA}$	$\lambda = 4358 \text{ \AA}$	Average
	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$
30	0.695	0.693	0.689	0.687	0.691
34	0.673	0.670	0.668	0.666	0.669
37	0.657	0.655	0.653	0.650	0.654
43	0.618	0.617	0.614	0.612	0.615
49	0.580	0.579	0.577	0.574	0.577
54	0.541	0.540	0.537	0.535	0.538
59	0.502	0.501	0.500	0.497	0.500
62	0.451	0.449	0.448	0.447	0.449
65	0.392	0.391	0.390	0.389	0.391
67	0.338	0.336	0.336	0.334	0.336

**Table 3.19**

**Order parameter  $\langle P_2 \rangle$  of sample BPPCC at different temperatures by Neugebauer method.**

$$(\alpha_{\parallel} - \alpha_{\perp}) = 12.50 \text{ in } 10^{-24} \text{ cm}^3 \text{ unit.}$$

Temp. in ° C	$\lambda = 6907 \text{ \AA}$	$\lambda = 5780 \text{ \AA}$	$\lambda = 5461 \text{ \AA}$	$\lambda = 4358 \text{ \AA}$	Average
	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$
43	0.632	0.630	0.629	0.626	0.629
48	0.610	0.607	0.607	0.604	0.607
51.5	0.595	0.594	0.593	0.590	0.593
55	0.581	0.580	0.578	0.574	0.578
60	0.547	0.546	0.545	0.542	0.545
63	0.507	0.506	0.505	0.502	0.505
68	0.467	0.466	0.465	0.462	0.465
70	0.383	0.382	0.380	0.378	0.381

**Table 3.20**

**Order parameter  $\langle P_2 \rangle$  of sample PPPCC at different temperatures by Neugebauer method.**

$$(\alpha_{\parallel} - \alpha_{\perp}) = 12.14 \text{ in } 10^{-24} \text{ cm}^3 \text{ unit.}$$

Temp. in °C	$\lambda = 6907 \text{ \AA}$	$\lambda = 5780 \text{ \AA}$	$\lambda = 5461 \text{ \AA}$	$\lambda = 4358 \text{ \AA}$	Average
	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$
33	0.647	0.644	0.643	0.641	0.644
36	0.644	0.642	0.641	0.638	0.641
38.4	0.641	0.639	0.637	0.635	0.638
42	0.637	0.635	0.633	0.631	0.634
46	0.628	0.626	0.624	0.622	0.625
49	0.621	0.619	0.618	0.615	0.618
52	0.614	0.612	0.610	0.607	0.611
56	0.599	0.597	0.595	0.593	0.596
60	0.585	0.584	0.581	0.580	0.583
64	0.567	0.564	0.564	0.562	0.564
67	0.553	0.552	0.551	0.549	0.551
71	0.494	0.493	0.492	0.489	0.492
74	0.431	0.429	0.429	0.427	0.429

**Table 3.21**

**Mean experimental intensity values  $I(\psi)$ , in arbitrary units, of CPPCC after background correction.**

$\psi$ ( degree )	$I(\psi)$ values at different temperatures in $^{\circ}\text{C}$				
	50	55	60	65	69
0	4.35	9.45	9.10	6.75	7.40
5	4.10	9.00	8.90	6.65	7.20
10	3.50	8.25	8.30	6.45	7.05
15	2.95	7.25	7.35	6.05	6.50
20	2.40	5.95	6.15	5.45	5.73
25	1.73	4.85	5.25	4.35	4.90
30	1.18	3.80	4.07	3.50	4.05
35	0.85	2.95	3.28	2.80	3.35
40	0.60	2.25	2.80	2.25	2.65
45	0.58	1.75	2.10	1.80	2.35
50	0.48	1.30	1.65	1.35	1.93
55	0.40	1.05	1.28	1.10	1.55
60	0.35	0.85	1.05	0.90	1.35
65	0.33	0.70	0.85	0.75	1.20
70	0.33	0.55	0.75	0.60	1.00
75	0.30	0.45	0.60	0.53	0.70
80	0.29	0.40	0.45	0.43	0.50
85	0.27	0.20	0.20	0.28	0.30
90	0.00	0.00	0.00	0.00	0.00

**Table 3.22****Normalised distribution function values  $f(\beta)$  of CPPCC**

$\beta$ ( degree )	$f(\beta)$ values at different temperatures in $^{\circ}$ C				
	50	55	60	65	69
0	9.11	6.96	5.71	4.12	4.11
5	8.76	6.84	5.80	4.30	4.22
10	7.72	6.32	5.71	4.61	4.35
15	6.15	5.27	4.95	4.54	4.10
20	4.48	4.02	3.76	3.90	3.44
25	3.07	3.02	2.78	3.08	2.75
30	2.05	2.35	2.23	2.43	2.25
35	1.34	1.84	1.89	1.93	1.88
40	0.86	1.34	1.50	1.46	1.47
45	0.57	0.90	1.03	1.03	1.06
50	0.42	0.59	0.67	0.71	0.76
55	0.35	0.43	0.49	0.53	0.62
60	0.34	0.37	0.43	0.45	0.59
65	0.33	0.32	0.40	0.39	0.56
70	0.31	0.25	0.32	0.31	0.44
75	0.25	0.16	0.19	0.21	0.27
80	0.18	0.09	0.10	0.12	0.13
85	0.14	0.06	0.06	0.08	0.07
90	0.13	0.05	0.04	0.07	0.06



**Table 3.24****Normalised distribution function values  $f(\beta)$  of CPBCC.**

$\beta$ (deg.)	$f(\beta)$ values at different temperatures in degrees								
	30.5	35	40	45	50	55	60	65	67.5
0	7.85	7.77	6.92	6.87	7.37	6.00	6.19	4.70	5.70
5	7.76	7.73	6.94	6.89	7.20	5.90	5.86	4.84	5.60
10	7.31	7.34	6.76	6.68	6.55	5.57	5.08	5.01	5.16
15	6.26	6.22	6.04	5.80	5.36	5.02	4.23	4.73	4.24
20	4.85	4.70	4.84	4.49	4.05	4.27	3.61	3.91	3.20
25	3.55	3.40	3.57	3.31	3.07	3.39	3.21	2.99	2.46
30	2.56	2.50	2.53	2.48	2.43	2.48	2.80	2.29	2.06
35	1.81	1.81	1.74	1.86	1.93	1.70	2.16	1.81	1.82
40	1.21	1.21	1.16	1.30	1.39	1.14	1.41	1.42	1.52
45	0.75	0.73	0.75	0.83	0.90	0.81	0.85	1.06	1.15
50	0.45	0.45	0.50	0.52	0.58	0.65	0.56	0.77	0.85
55	0.29	0.31	0.37	0.37	0.42	0.57	0.46	0.58	0.70
60	0.20	0.25	0.28	0.30	0.36	0.51	0.46	0.47	0.65
65	0.14	0.21	0.21	0.24	0.30	0.39	0.44	0.37	0.57
70	0.09	0.14	0.13	0.17	0.21	0.24	0.32	0.27	0.39
75	0.05	0.07	0.07	0.09	0.10	0.12	0.16	0.18	0.19
80	0.03	0.03	0.03	0.04	0.05	0.06	0.07	0.11	0.08
85	0.02	0.01	0.02	0.03	0.02	0.03	0.03	0.07	0.04
90	0.01	0.01	0.02	0.02	0.02	0.03	0.02	0.06	0.03



**Table 3.26****Normalised distribution function values  $f(\beta)$  of BPPCC.**

$\beta$ (deg.)	$f(\beta)$ values at different temperatures in degrees						
	45	50	55	60	65	70	72
0	7.14	7.31	5.84	4.95	6.47	4.28	4.21
5	7.32	7.25	5.81	5.02	6.19	4.45	4.08
10	7.47	6.90	5.64	5.08	5.51	4.66	3.76
15	6.76	6.02	5.17	4.84	4.66	4.35	3.43
20	5.10	4.70	4.42	4.22	3.87	3.51	3.16
25	3.35	3.36	3.55	3.40	3.15	2.71	2.93
30	2.12	2.29	2.69	2.59	2.45	2.23	2.60
35	1.38	1.52	1.90	1.87	1.76	1.95	2.12
40	0.94	1.01	1.26	1.29	1.17	1.60	1.56
45	0.66	0.70	0.81	0.87	0.76	1.15	1.06
50	0.47	0.53	0.54	0.61	0.54	0.78	0.75
55	0.36	0.45	0.40	0.47	0.45	0.58	0.62
60	0.30	0.40	0.33	0.40	0.42	0.50	0.58
65	0.25	0.32	0.27	0.34	0.41	0.46	0.10
70	0.19	0.22	0.20	0.26	0.36	0.37	0.52
75	0.14	0.12	0.13	0.18	0.27	0.22	0.42
80	0.09	0.06	0.08	0.11	0.19	0.11	0.28
85	0.07	0.04	0.06	0.08	0.14	0.07	0.15
90	0.06	0.03	0.05	0.07	0.12	0.05	0.05



**Table 3.28****Normalised distribution function values  $f(\beta)$  of PPPCC.**

$\beta$ (deg.)	$f(\beta)$ values at different temperatures in degrees							
	40	45	50	55	60	65	70	74
0	12.14	7.81	6.63	7.81	11.47	4.42	5.35	3.65
5	11.72	7.96	6.57	7.44	11.14	4.49	5.18	3.83
10	10.03	7.83	6.24	6.47	9.37	4.58	4.68	4.17
15	7.06	6.55	5.44	5.27	6.07	4.41	3.96	4.18
20	4.24	4.57	4.37	4.14	3.23	3.94	3.28	3.65
25	2.54	2.99	3.41	3.22	1.84	3.34	2.84	2.92
30	1.74	2.11	2.67	2.45	1.41	2.72	2.58	2.32
35	1.33	1.62	2.01	1.76	1.37	2.06	2.26	1.86
40	0.98	1.20	1.37	1.18	1.30	1.39	1.72	1.45
45	0.64	0.81	0.84	0.78	1.00	0.87	1.12	1.08
50	0.41	0.53	0.52	0.55	0.66	0.57	0.70	0.82
55	0.30	0.39	0.36	0.44	0.50	0.44	0.50	0.69
60	0.28	0.33	0.29	0.39	0.49	0.41	0.41	0.62
65	0.28	0.28	0.24	0.33	0.51	0.40	0.37	0.54
70	0.25	0.19	0.16	0.24	0.39	0.34	0.30	0.37
75	0.16	0.09	0.09	0.15	0.19	0.23	0.20	0.19
80	0.08	0.04	0.04	0.08	0.06	0.13	0.12	0.09
85	0.05	0.02	0.02	0.05	0.02	0.08	0.07	0.04
90	0.04	0.01	0.02	0.04	0.01	0.06	0.06	0.03

**Table 3.29****Sample : CPPCC****Variation of  $\langle P_2 \rangle$  and  $\langle P_4 \rangle$  with temperature.**

Temperature in ° C	$\langle P_2 \rangle$	$\langle P_4 \rangle$
50	0.579	0.297
55	0.561	0.207
60	0.522	0.167
65	0.502	0.140
69	0.453	0.112

**Table 3.30****Sample : CPBCC****Variation of  $\langle P_2 \rangle$  and  $\langle P_4 \rangle$  with temperature.**

Temperature in ° C	$\langle P_2 \rangle$	$\langle P_4 \rangle$
30.5	0.656	0.274
35	0.641	0.268
40	0.629	0.253
45	0.609	0.234
50	0.585	0.211
55	0.553	0.190
60	0.531	0.158
65	0.511	0.147
67.5	0.470	0.115

**Table 3.31****Sample : BPPCC****Variation of  $\langle P_2 \rangle$  and  $\langle P_4 \rangle$  with temperature.**

Temperature in ° C	$\langle P_2 \rangle$	$\langle P_4 \rangle$
45	0.618	0.288
50	0.600	0.253
55	0.579	0.207
60	0.540	0.177
65	0.512	0.196
70	0.477	0.118
72	0.450	0.086

**Table 3.32****Sample : PPPCC****Variation of  $\langle P_2 \rangle$  and  $\langle P_4 \rangle$  with temperature.**

Temperature in ° C	$\langle P_2 \rangle$	$\langle P_4 \rangle$
40	0.640	0.345
45	0.620	0.264
50	0.605	0.219
55	0.576	0.225
60	0.557	0.257
65	0.515	0.156
70	0.498	0.121
74	0.471	0.104

**Table 3.33****Apparent molecular length ( $l_{ap}$ ) at different temperature.**Sample to film distance = 4.46 cm.,  $\lambda = 1.54051 \text{ \AA}$ ,

Magnetic field = 5 K. Gauss

Sample: CPPCC				
Temp. in °C	$l_{ap}$ in $\text{\AA}$	Mean $l_{ap}$ in $\text{\AA}$	Model length L in $\text{\AA}$	$l_{ap}/L$
50	22.62	22.66	16.3	1.39
55	22.59			
60	22.8			
65	22.86			
69	22.93			

**Table 3.34****Apparent molecular length ( $l_{ap}$ ) at different temperature.**Sample to film distance = 4.46 cm.,  $\lambda = 1.54051 \text{ \AA}$ ,

Magnetic field = 5 K. Gauss

Sample: CPBCC				
Temp. in °C	$l_{ap}$ in $\text{\AA}$	Mean $l_{ap}$ in $\text{\AA}$	Model length L in $\text{\AA}$	$l_{ap}/L$
30.5	24.38	24.42	17.2	1.42
35	24.42			
40	24.5			
45	24.42			
50	24.5			
55	24.54			
60	24.53			
65	24.52			
67.5	24.54			

**Table 3.35****Apparent molecular length ( $l_{ap}$ ) at different temperature.**Sample to film distance = 4.46 cm.,  $\lambda = 1.54051 \text{ \AA}$ ,

Magnetic field = 5 K. Gauss

Sample: BPPCC				
Temp. in °C	$l_{ap}$ in $\text{\AA}$	Mean $l_{ap}$ in $\text{\AA}$	Model length L in $\text{\AA}$	$l_{ap}/L$
45	20.7	20.87	19.15	1.09
50	20.77			
55	20.7			
60	20.79			
65	20.82			
70	21.04			
72	21.23			

**Table 3.36****Apparent molecular length ( $l_{ap}$ ) at different temperature.**Sample to film distance = 4.46 cm.,  $\lambda = 1.54051 \text{ \AA}$ ,

Magnetic field = 5 K. Gauss

Sample: PPPCC				
Temp. in °C	$l_{ap}$ in $\text{\AA}$	Mean $l_{ap}$ in $\text{\AA}$	Model length L in $\text{\AA}$	$l_{ap}/L$
37	23.98	24.26	21.1	1.15
40	23.92			
45	24.08			
50	23.98			
55	24.11			
60	24.24			
65	24.14			
70	24.21			
74.5	24.43			

**Table 3.37**

**Experimental values of the density ( $\rho$ ), magnetic susceptibility ( $\chi$ ), susceptibility anisotropy ( $\Delta\chi$ ), and the order parameter  $\langle P_2 \rangle$ .**

**Sample: CPPCC**

Temp. in °C	Density ( $\rho$ ) in gm/cc	$-\chi_{\parallel} \times 10^{-7}$ c.g.s.unit	$\Delta\chi \times 10^{-8}$ c.g.s.unit	order parameter $\langle P_2 \rangle$
48.5	1.069	6.85	4.8	0.590
52.5	1.067	6.87	4.7	0.570
58.5	1.062	6.88	4.4	0.535
63.0	1.057	6.91	4.0	0.488
67.5	1.051	6.95	3.4	0.420
75.0	1.040	$7.18 = \bar{\chi}_{iso}$		

$$\Delta\chi_o = 8.22 \times 10^{-8} \text{ c.g.s.unit ;}$$

**Table 3.38**

**Experimental values of the density ( $\rho$ ), magnetic susceptibility ( $\chi$ ), susceptibility anisotropy ( $\Delta\chi$ ), and the order parameter  $\langle P_2 \rangle$ .**

**Sample: CPBCC**

Temp. in °C	Density ( $\rho$ ) in gm/cc	$-\chi_{\parallel} \times 10^{-7}$ c.g.s.unit	$\Delta\chi \times 10^{-8}$ c.g.s.unit	order parameter $\langle P_2 \rangle$
38.5	1.044	6.71	5.0	0.643
43.0	1.041	6.72	4.8	0.613
48.0	1.036	6.74	4.6	0.582
53.0	1.034	6.75	4.4	0.558
58.5	1.026	6.77	4.1	0.523
63.0	1.022	6.80	3.6	0.462
67.0	1.016	6.84	3.1	0.393
75.0	1.004	$7.05 = \bar{\chi}_{\text{iso}}$		

$$\Delta\chi_0 = 7.85 \times 10^{-8} \text{ c.g.s.unit};$$

**Table 3.39**

**Experimental values of the density ( $\rho$ ), magnetic susceptibility ( $\chi$ ), susceptibility anisotropy ( $\Delta\chi$ ), and the order parameter  $\langle P_2 \rangle$ .**

**Sample: BPPCC**

Temp. in ° C	Density ( $\rho$ ) in gm/cc	$-\chi_{\parallel} \times 10^{-7}$ c.g.s.unit	$\Delta\chi \times 10^{-8}$ c.g.s.unit	order parameter $\langle P_2 \rangle$
44.0	0.992	6.24	3.8	0.626
49.0	0.988	6.25	3.6	0.594
54.0	0.984	6.27	3.4	0.567
59.0	0.980	6.28	3.2	0.535
63.0	0.976	6.29	3.1	0.509
67.5	0.972	6.32	2.6	0.430
70.5	0.969	6.35	2.2	0.370
78.0	0.960	$6.49 = \bar{\chi}_{iso}$		

$$\Delta\chi_o = 6.04 \times 10^{-8} \text{ c.g.s.unit ;}$$

**Table 3.40**

**Experimental values of the density ( $\rho$ ), magnetic susceptibility ( $\chi$ ), susceptibility anisotropy ( $\Delta\chi$ ), and the order parameter  $\langle P_2 \rangle$ .**

**Sample: PPPCC**

Temp. in °C	Density ( $\rho$ ) in gm/cc	$-\chi_{\parallel} \times 10^{-7}$ c.g.s.unit	$\Delta\chi \times 10^{-8}$ c.g.s.unit	order parameter $\langle P_2 \rangle$
39.0	0.975	6.34	4.0	0.644
43.0	0.973	6.35	3.9	0.627
48.0	0.968	6.36	3.8	0.600
53.0	0.964	6.37	3.6	0.575
58.5	0.960	6.38	3.4	0.546
62.0	0.956	6.38	3.3	0.535
67.0	0.952	6.43	3.1	0.493
71.0	0.948	6.45	2.8	0.450
74.0	0.944	6.48	2.6	0.411
81.0	0.938	$6.61 = \bar{\chi}_{iso}$		

$$\Delta\chi_o = 6.27 \times 10^{-8} \text{ c.g.s.unit ;}$$

**Table 3.41**

**Experimental values of splay elastic constant ( $K_{11}$ ) for various ( $T_c - T$ ) values.**

**Sample: CPPCC**

$T_c = 70^\circ \text{C}$ , Sample thickness = 162  $\mu\text{m}$ ,  $H_c$  = Threshold magnetic field

$T_c - T$	$H_c$ in Gauss	$\Delta\chi \times 10^{-8}$ cgs unit	$K_{11} \times 10^{-6}$ dyne
1	715	3.3	0.45
6	750	3.9	0.58
11	770	4.4	0.69
15.5	790	4.6	0.77
21	815	4.9	0.86

**Table 3.42**

**Experimental values of bend elastic constant ( $K_{33}$ ) for various ( $T_c - T$ ) values.**

**Sample: CPPCC**

$T_c = 70^\circ \text{C}$ , Sample thickness = 162  $\mu\text{m}$ ,  $H_c$  = Threshold magnetic field

$T_c - T$	$H_c$ in Gauss	$\Delta\chi \times 10^{-8}$ cgs unit	$K_{33} \times 10^{-6}$ dyne
1	750	3.3	0.49
6	805	3.9	0.67
11	860	4.4	0.86
15.5	900	4.6	1.00
21	960	4.9	1.20

**Table 3.43**

**Experimental values of splay elastic constant ( $K_{11}$ ) for various ( $T_c - T$ ) values.**

**Sample: CPBCC**

$T_c = 68.3^\circ \text{C}$ , Sample thickness = 162  $\mu\text{m}$ ,  $H_c$  = Threshold magnetic field

$T_c - T$	$H_c$ in Gauss	$\Delta\chi \times 10^{-8}$ cgs unit	$K_{11} \times 10^{-6}$ dyne
1.3	624	3.1	0.32
6.3	660	3.8	0.44
11.3	670	4.2	0.51
16.3	675	4.5	0.54
21.3	685	4.6	0.59
26.3	710	4.7	0.63
30.3	711	5.2	0.69
34.8	720	5.4	0.75

**Table 3.44**

**Experimental values of bend elastic constant (  $K_{33}$  ) for various  
( $T_c - T$ ) values.**

**Sample: CPBCC**

$T_c = 68.3^\circ \text{C}$  , Sample thickness = 162  $\mu\text{m}$ ,  $H_c$  = Threshold magnetic field

$T_c - T$	$H_c$ in Gauss	$\Delta\chi \times 10^{-8}$ cgs unit	$K_{33} \times 10^{-6}$ dyne
1.3	626	3.1	0.32
6.3	666	3.8	0.44
11.3	686	4.2	0.53
16.3	706	4.5	0.59
21.3	726	4.7	0.66
26.3	756	4.7	0.72
30.3	760	5.2	0.80
34.8	786	5.4	0.89

**Table 3.45**

**Experimental values of splay elastic constant ( $K_{11}$ ) for various ( $T_c - T$ ) values.**

**Sample: BPPCC**

$T_c = 72.6^\circ \text{C}$  , Sample thickness = 101  $\mu\text{m}$ ,  $H_c$  = Threshold magnetic field

$T_c - T$	$H_c$ in Gauss	$\Delta\chi \times 10^{-8}$ cgs unit	$K_{11} \times 10^{-6}$ dyne
2.6	1030	2.3	0.25
4.6	1080	2.5	0.30
9.6	1120	3.1	0.40
14.6	1160	3.3	0.45
19.6	1210	3.4	0.52
24.6	1230	3.6	0.57
29.1	1260	3.8	0.62

**Table3.46**

**Experimental values of bend elastic constant ( $K_{33}$ ) for various  
( $T_c - T$ ) values.**

**Sample: BPPCC**

$T_c = 72.6^\circ \text{C}$ , Sample thickness = 101  $\mu\text{m}$ ,  $H_c$  = Threshold magnetic field

$T_c - T$	$H_c$ in Gauss	$\Delta\chi \times 10^{-8}$ cgs unit	$K_{33} \times 10^{-6}$ dyne
2.6	960	2.3	0.22
4.6	1000	2.5	0.26
9.6	1050	3.1	0.35
14.6	1120	3.3	0.42
19.6	1170	3.4	0.49
24.6	1200	3.6	0.54
29.1	1230	3.8	0.59

**Table 3.47**

**Experimental values of splay elastic constant ( $K_{11}$ ) for various ( $T_c - T$ ) values.**

**Sample: PPPCC**

$T_c = 75.0^\circ \text{C}$  ; Sample thickness = 162  $\mu\text{m}$ ,  $H_c$  = Threshold magnetic field

$T_c - T$	$H_c$ in Gauss	$\Delta\chi \times 10^{-8}$ cgs unit	$K_{11} \times 10^{-6}$ dyne
1	820	2.6	0.46
5.5	880	2.9	0.60
10	950	3.2	0.77
15	1000	3.3	0.88
20	1060	3.5	1.06
25	1120	3.7	1.23
30	1230	3.9	1.55
35	1330	4.0	1.89

**Table 3.48**

**Experimental values of splay elastic constant ( $K_{33}$ ) for various ( $T_c - T$ ) values.**

**Sample: PPPCC**

$T_c = 75.0^\circ \text{C}$ , Sample thickness = 162  $\mu\text{m}$ ,  $H_c$  = Threshold magnetic field

$T_c - T$	$H_c$ in Gauss	$\Delta\chi \times 10^{-8}$ cgs unit	$K_{33} \times 10^{-6}$ dyne
1	819	2.6	0.46
5.5	870	2.9	0.59
10	920	3.2	0.72
15	950	3.3	0.79
20	980	3.5	0.90
25	1010	3.7	1.00
30	1085	3.9	1.21
35	1160	4.0	1.44

**Table 3.49**

**Experimental values of the Frank elastic constant ratio ( $K_{33} / K_{11}$ ) at different relative temperatures ( $T_c - T$ ).**

Sample: CPPCC		Sample: CPBCC	
$T_c - T$	$K_{33} / K_{11}$	$T_c - T$	$K_{33} / K_{11}$
1	1.10	1.3	1.01
6	1.15	6.3	1.02
11	1.25	11.3	1.05
15.5	1.30	16.3	1.09
21	1.39	21.3	1.12
		26.3	1.13
		30.3	1.14
		34.8	1.19

**Table 3.50**

**Experimental values of the Frank elastic constant ratio ( $K_{33} / K_{11}$ ) at different relative temperatures ( $T_c - T$ ).**

Sample: BPPCC		Sample: PPPCC	
$T_c - T$	$K_{33} / K_{11}$	$T_c - T$	$K_{33} / K_{11}$
2.6	0.87	1	1.00
4.6	0.87	5.5	0.98
9.6	0.88	10	0.94
14.6	0.93	15	0.90
19.6	0.93	20	0.86
24.6	0.95	25	0.81
29.1	0.95	30	0.78
		35	0.76

**References:**

- 1) Hoffmann-La Roche Catalogue.
- 2) M. Takahashi, S. Mita and S. Kondo, *Mol. Cryst. Liq. Cryst.*, 132, 53 (1986).
- 3) M. Mitra, S. Paul and R. Paul, *Pramana-J. Phys.*, 29, 409 (1987).
- 4) A. J. Leadbetter, R. M. Richardson and C. N. Colling, *J. Phys.*, (Paris) 36, 1 (1975).
- 5) R. Chang, *Mol. Cryst. Liq. Cryst.*, 30, 155 (1975).
- 6) D. Revannasiddaiah and D. Krishnamurti, *Mol. Cryst. Liq. Cryst.*, 53, 63 (1979).
- 7) I. H. Ibrahim and W. Hasse, *J. de Physique*, C3, 40, C3-164 (1979).
- 8) I. H. Ibrahim and W. Hasse, *Z. Naturforsch.*, 31a, 1644 (1976).
- 9) M. Mitra and R. Paul, *Mol. Cryst. Liq. Cryst.*, 148, 185 (1987).
- 10) A. Scharkowski, H. Schmiedel, R. Stannarius and E. Weissshuhn, *Mol. Cryst. Liq. Cryst.*, 191, 419 (1990).
- 11) M. Schadt, R. Buchecker, F. Leenhouts, A. Boller, *Mol. Cryst. Liq. Cryst.*, 139, 1 (1986).
- 12) M. J. Bradshaw, E. P. Raynes, I. Fedak and A. J. Leadbetter, *J. Physique*, 45, 157 (1984).