# CHAPTER 6

Study of mesomorphic properties of three alkenyl liquid crystalline compounds.

6.1 INTRODUCTION

As the complexity and diversity of the liquid crystal display technology increases, demands for new liquid crystal materials with wide band-width of material properties also increases. New type of polar and non-polar bicyclohexane liquid crystals containing alkenyl side chains were reported in this context[1-4]. These compounds have low optical anisotropy, low viscosity but high elastic constants, so can be used in display devices as materials of short response times. Properties of these compounds changes markedly with respect to the position of the double bond in the alkenyl chain. Since the end chains in nematics are usually quite short, double bonds are close to the core and steric interactions between the core and the double bonds are certainly important. In view of these I have undertaken the study of some alkenyl liquid crystalline compounds which have nematic phase over a wide range.

In this chapter the experimental result of x-ray diffraction and optical studies on three compounds having the following structures have been discussed,

$$C_nH_{2n-1}-\langle H \rangle - \langle H \rangle - R$$
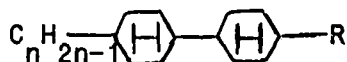
(I)   n=3, R=CN, 4(1″-propenyl)4′(cyano)1,1′ bicyclohexane.
      [1d(1)CC].

(II) n=5, R=CN, 4(3″-pentenyl)4′(cyano)1,1′ bicyclohexane
      [1d(3)CC].

(III) n=5, R=OC$_2$H$_5$, 4(3″-pentenyl)4′(ethoxy)1,1′ bicyclohexane.
      [1d(3)CCO2]

The crystal structure for the compounds 1d(3)CC and 1d(3)CCO2 has already been solved[5,6] and discussed in chapter 3 and chapter 4.

6.2 EXPERIMENTAL DETAILS

6.2.1 Texture Study

The phase transition of the three compounds were studied by observing textures under crossed polarizers with a polarising microscope of magnification 150x. The transition temperatures agree well with the literature values, except that we get supercooling in all three compounds and for 1d(3)CC we observed smecticA phase for a very short range of temperature during cooling. The compounds 1d(1)CC and 1d(3)CCO2 showed marbled textures, both during heating and cooling, which are often found in the nematic phase. The compound 1d(3)CC showed a fan shaped texture of SmecticA phase and a nematic marbled texture. The existence of these phases were also confirmed from x-ray studies.

6.2.2 X-ray diffration study

A detailed description of the experimental method for x-ray diffraction study is given in chapter 5. The alkenyl bicyclohexanes under investigation have very small magnetic anisotropy, virtually zero[4] and these could not be aligned by usual magnetic field. By heating the sample slowly to the isotropic state and then cooling it down to the desired temperature well aligned samples were obtained. Diffraction photographs were taken at regular intervals during cooling from isotropic phase.

In order to determine the various parameters, the photographs were scanned, both linearly and circularly, by an optical micro densitometer (VEB Carl Zeiss Jena, Model MD 100) equiped with an automatic recording facility. The measured optical densities were converted to x-ray intensity values with the help of a calibration curve following Klug and Alexander[7].

To obtain better accuracy in the layer thickness measurement, x-ray diffraction photographs of inner rings were taken, increasing the sample to film distance about 9cm with a Carl Zeiss Universal

Camera (Model 90486) for the compound 1d(3)CC. The same measurements could not be done for the compound 1d(1)CC due to shut down of the x-ray generator.
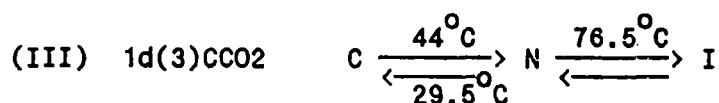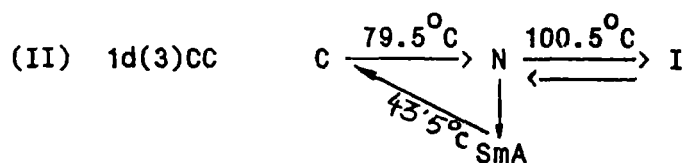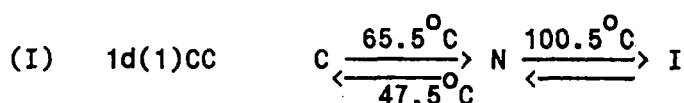
6.2.3 Optical study :

Birefringence measurements were made using the technique of thin prism and the experimental procedures were described in chapter 5. A precision spectrometer and a nicol prism were used to measure the refractive indices (n_o, n_e) within experimental error $\pm.001$ for three different wavelengths.

6.2.4 Density measurement :

The densities of the sample were determined by a dilatometer of capillary type. Temperature during the experiment was controlled to about $\pm 0.5^{\circ}C$ by a temperature controller. The experimental uncertainty of density measurement is 1%.

6.3 RESULTS AND DISCUSSIONS

From texture study, the three compounds are found to have the following mesophase behaviour,

(I) 1d(1)CC $\quad C \xrightarrow[\xleftarrow{47.5^{\circ}C}]{65.5^{\circ}C} N \xrightarrow[\longleftarrow]{100.5^{\circ}C} I$

(II) 1d(3)CC $\quad C \xrightarrow{79.5^{\circ}C} N \xrightarrow[\longleftarrow]{100.5^{\circ}C} I$

$\quad\quad\quad\quad\quad\quad\quad\quad 43.5^{\circ}C \searrow \quad\downarrow$

$\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad SmA$

(III) 1d(3)CCO2 $\quad C \xrightarrow[\xleftarrow{29.5^{\circ}C}]{44^{\circ}C} N \xrightarrow[\longleftarrow]{76.5^{\circ}C} I$

6.3.1 Refractive index measurements

Variations of density measurements with temperatures for the

samples are given in figure 6.1. The density graph for the compound 1d(3)CC shows a first order phase transition at $45^{\circ}c$ in the supercooled state. The phase was identified to be SmA by our x-ray and texture studies. Figures 6.2 - 6.4 indicate the variation of (n_o, n_e) with temperature of the three samples. The refractive indices (n_o, n_e) and the densities of the three samples at different temperatures for the three wave-lengths are arranged in tables 6.1 - 6.3.

It is found that the value of birefringence(Δn) is very low for these compounds. This low anisotropy may be due to the influence of the π-electron in -c=c- double bond of the alkenyl side chain which for all the three compounds are in even position making angles with the long axis of the molecule. Over and above this, the cyclohexane cores are less polarizable compared to the biphenyl cores. It will be interesting to study the optical anisotropy of compounds having double bonds in the odd positions.

From the values of the refractive indices the molecular polarizabilities (α_o, α_e) were calculated using Vuks[8] isotropic (1966) and Neugebauer's (1954) anisotropic[9] internal field models. The values of effective polarizabilities α_o and α_e obtained from Vuk's and Neugebauer's method are given in tables 6.4 - 6.6 and 6.7 - 6.9 respectively. From these polarizabily anisotropy values at different temperatures we calculated the orientational order parameter $\langle P_2 \rangle$ for all the three compounds. The values of order parameters $\langle P_2 \rangle$ at different temperatures obtained from the three different wavelengths and their average values have been included in tables 6.10 - 6.12 and 6.13 - 6.15. Due to lack of refractive index data in the crystalline state the values of $\alpha_{\parallel}$ and $\alpha_{\perp}$ could not be calculated directly. In order to obtain ($\alpha_{\parallel} - \alpha_{\perp}$) we took help of Haller's extrapolation procedure.

Estimation of the polarizabilities of the molecules was also carried out using the additive rule of bond polarizability proposed

by Le Fevre[10] (1965). This molar polarizability is approximated as a sum of bond polarizabilities

$$a = \sum a_k$$

the summation extending over all covalent bonds k in the molecule. Assuming rotational symmetry[11] around the bonds, a_k is specified by its longitudinal component ($\alpha_{\parallel}$) its transverse component ($\alpha_{\perp}$) and the orientations of the bond. The bond polarizability values were taken from Le Fevre.

Table 1.16 shows the experimental and calculated values of mean

TABLE - 6.16

Comparison of experimental and calculated polarizability values.

Compounds.	α		$\Delta\alpha$		
	Calculated	Expt.	Calculated	Experimental.	
				Vuks	Neug.
1d(1)CC	27.96	22.14	8.31	6.89	5.81
1d(3)CC	31.54	24.53	10.52	9.92	8.49
1d(3)CCO2	33.57	27.32	8.04	9.97	8.76

α and $\Delta\alpha$ are in 10^{-24} cm^3 unit.

polarizability α and molecular polarizability anisotropy $\Delta\alpha$. Since α_0 and α_e values at different wavelengths are quite close we have given values for $\lambda=5780\overset{o}{A}$ only.

It cannot be said that the experimental values of α agree well with calculated values. But it is observed that as the experimental values of α increases, the calculated values also increases. The calculated value of $\Delta\alpha$ for the compound 1d(1)CC and 1d(3)CC agree better with Vuk's values. For the third non-polar compound the
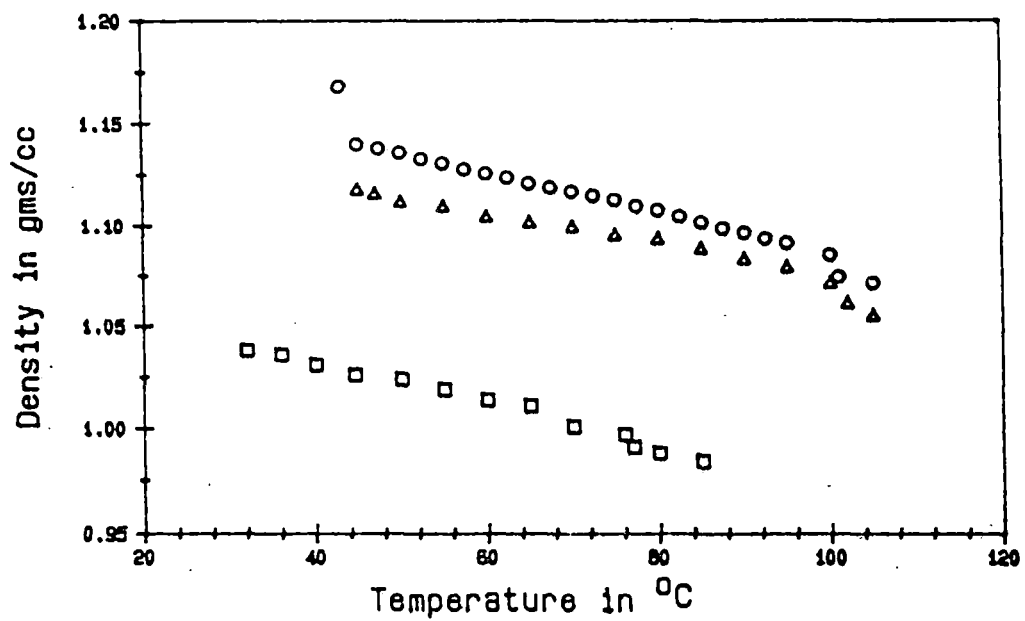
Figure 6.1 : Variation of density with temperature.
o - 1d(3)CC, Δ - 1d(1)CC, □ - 1d(3)CCO2.
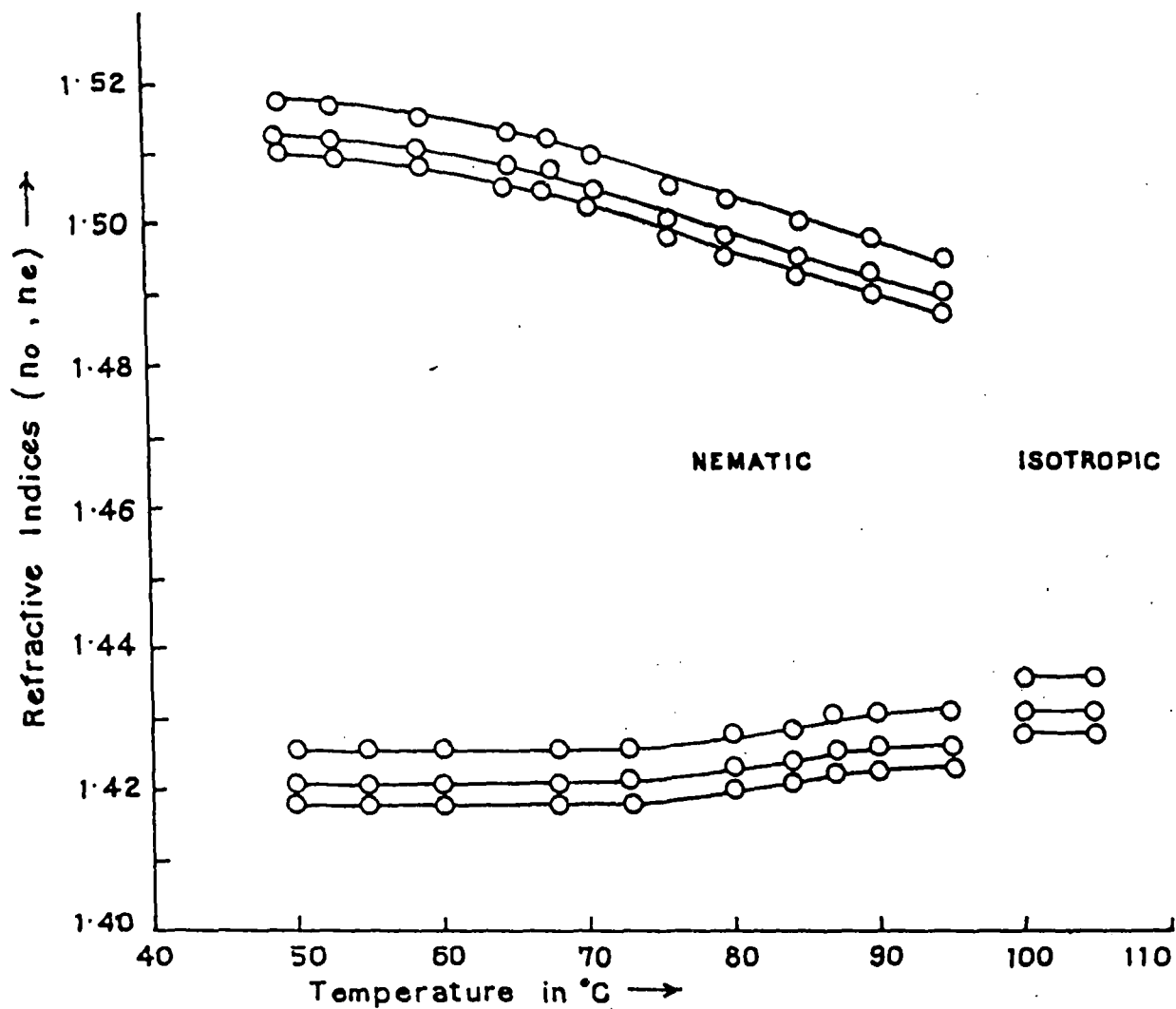
Figure 6.2 : Variation of refractive indices (n_o, n_e) at different temperatures of compound 1d(1)CC. Upper curve for λ = 5461 Å, middle curve for λ = 5780 Å, and lower curve for λ = 6907 Å.
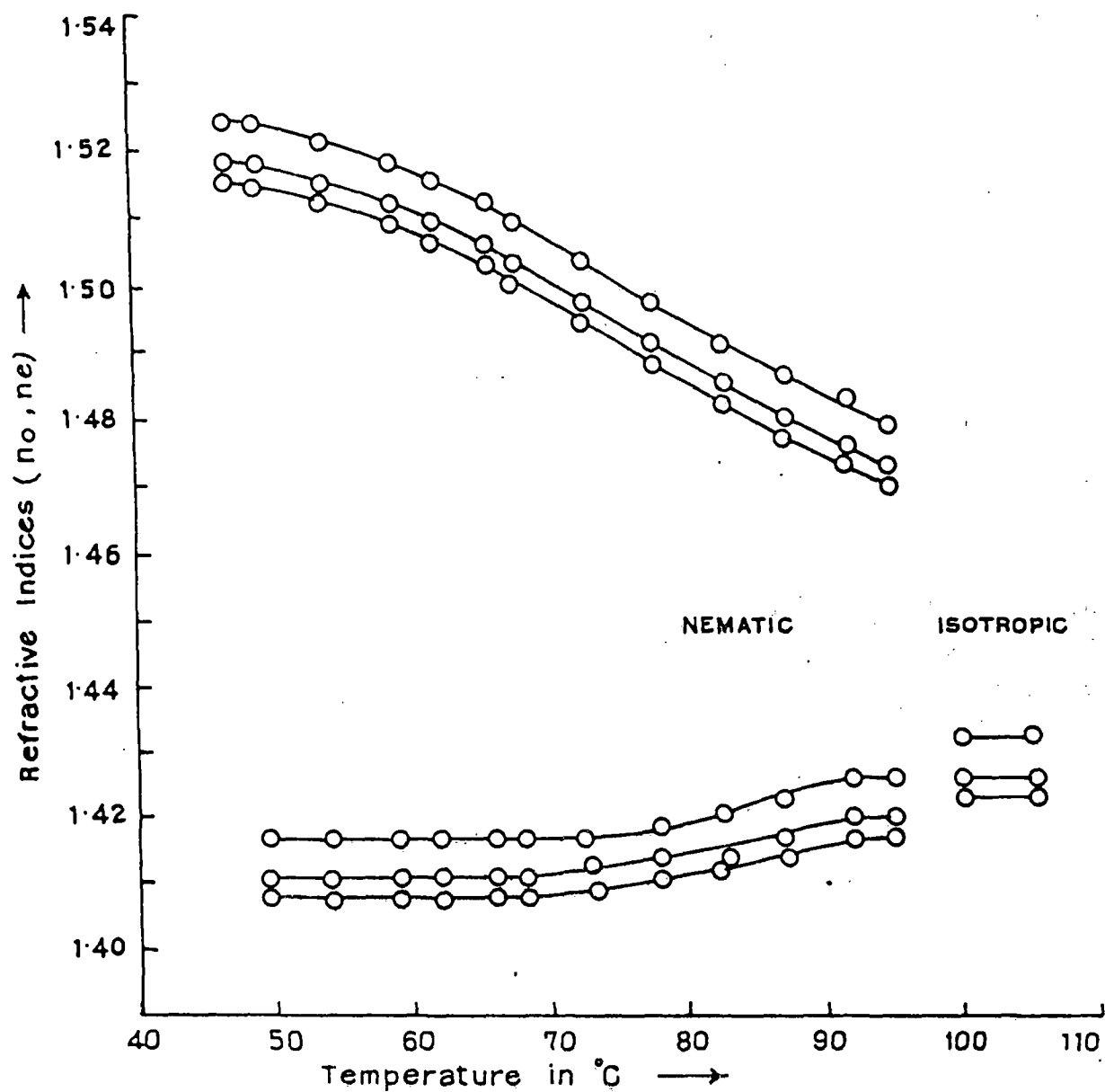
Figure 6.3 : Variation of refractive indices (n_o, n_e) at different temperatures of compound 1d(3)CC. Upper curve for λ = 5461 Å, middle curve for λ = 5780 Å, and lower curve for λ = 6907 Å.

Figure 6.4 : Variation of refractive indices (n_o, n_e) at different temperatures of compound 1d(3)CCO2 Upper curve for λ = 5461 $\overset{o}{A}$, middle curve for λ = 5780 $\overset{o}{A}$, and lower curve for λ = 6907 $\overset{o}{A}$.

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agreement is better with Neugebauer's. I could not arrive at any definite conclusion for this type of results, because all the three compounds do not belong to the same homologous series. Moreover, both additive rule 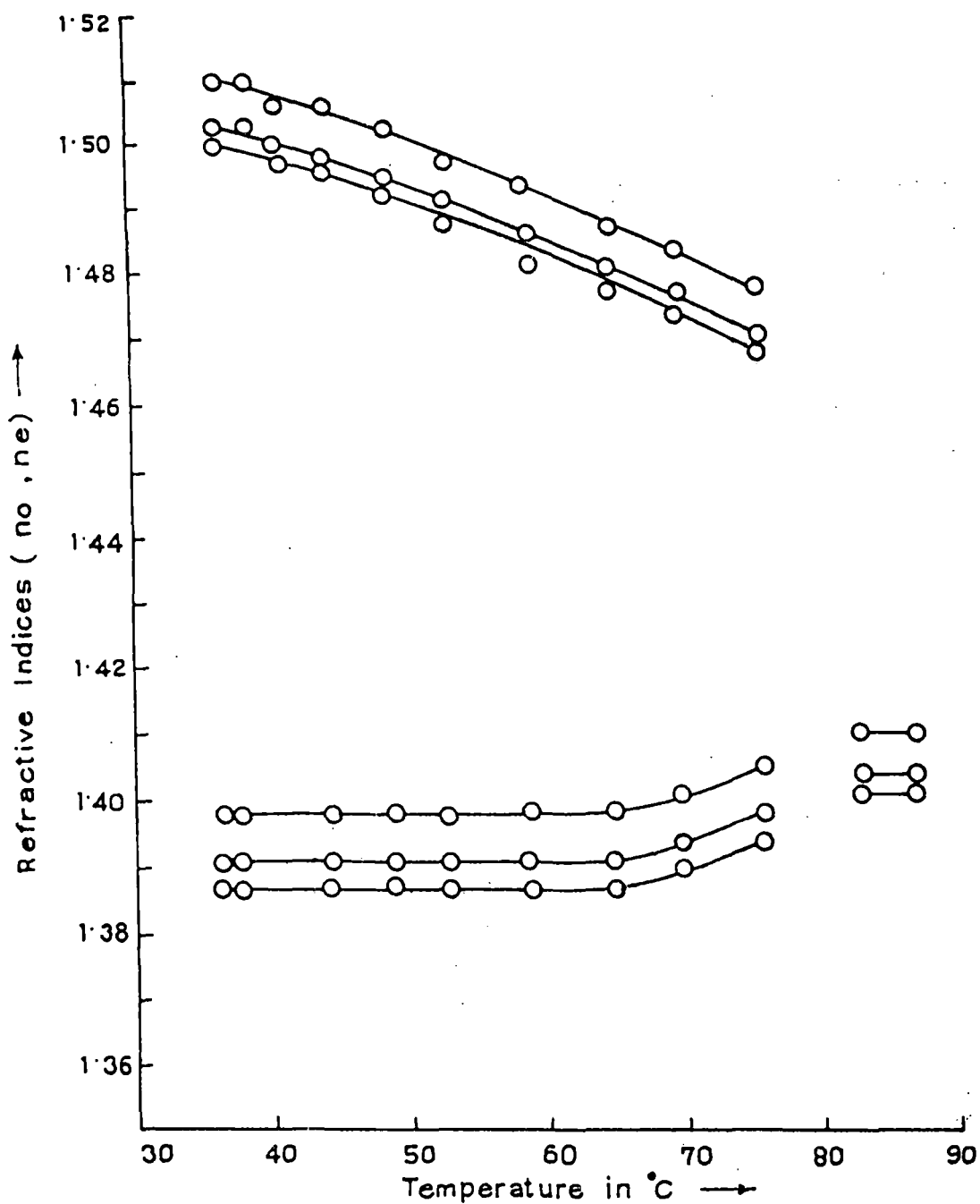of bond polarizability and Haller's extrapolation procedure is not free from limitations. Probably best results could have been obtained if experimental values of $\alpha_{\parallel}$ and $\alpha_{\perp}$ were available in the solid phase and then from comparison it could have been said definitely whether the extrapolation procedure is justified or not.

6.3.2 Parameters from x-ray diffraction study.

X-ray diffraction photographs of the three compounds at different temperatures are given in figures 6.5 - 6.10. From the x-ray diffraction photographs, fluctuation wave lengths[12] parallel and perpendicular to the director and correlation lengths for all the compounds have been calculated. X-ray intensity data from linear scanning of outer halo were fitted to a gaussian form[13] with a background varying linearly with the scattering vector q as follows,

$$I(q) = a + exp\{-b(q-c)^2\} + d + eq$$

The best fitted values of q_o, the peak position, give the value of intermolecular distance D using the relation D = $2\pi(1.117/q_o)$. The intensity vs q-values graph at temperature 50^oC for the compound 1d(3)CC is shown in the figure 6.11. The D values are found to be temperature independent for all the compounds. From the the best fitted value of Δq we calculated the correlation length and it has been found that the local director is random beyond five molecular diameters.

Fluctuation wavelength l parallel to the director are obtained from scattering about the meridional direction. using Bragg's formula. For 1d(3)CC this pseudo layer spacings in the nematic phase is about 1.8 times the molecular length (16Å). Antiparallel

Figure 6.5 : X-ray diffraction photograph of oriented sample 1d(1)CC at 77°C

Figure 6.6 : X-ray diffraction photograph of oriented sample 1d(1)CC at 85°C.

Figure 6.7 : X-ray diffraction photograph of oriented sample 1d(3)CC at 60°C.

Figure 6.8 : X-ray diffraction photograph of oriented sample 1d(3)CC at 45°C. (Smectic phase)
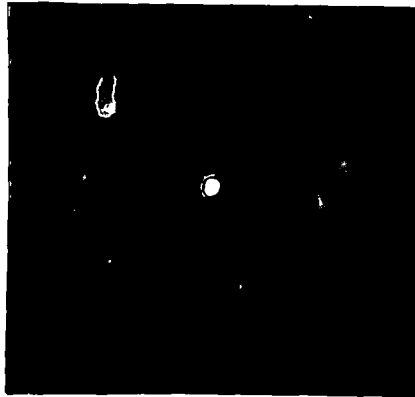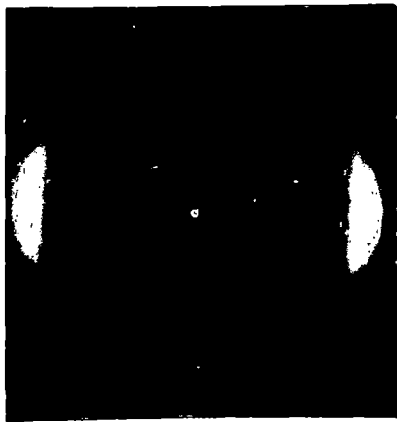
Figure 6.9 : X-ray diffraction photograph of oriented sample
1d(3)CCO2 at 35°C.
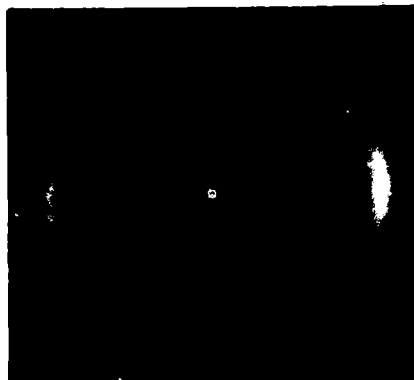
Figure 6.10 : X-ray diffraction photograph of oriented sample
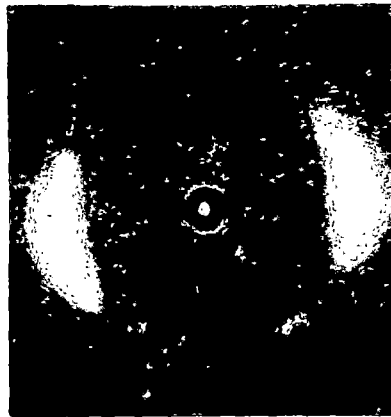1d(3)CCO2 at 60°C.
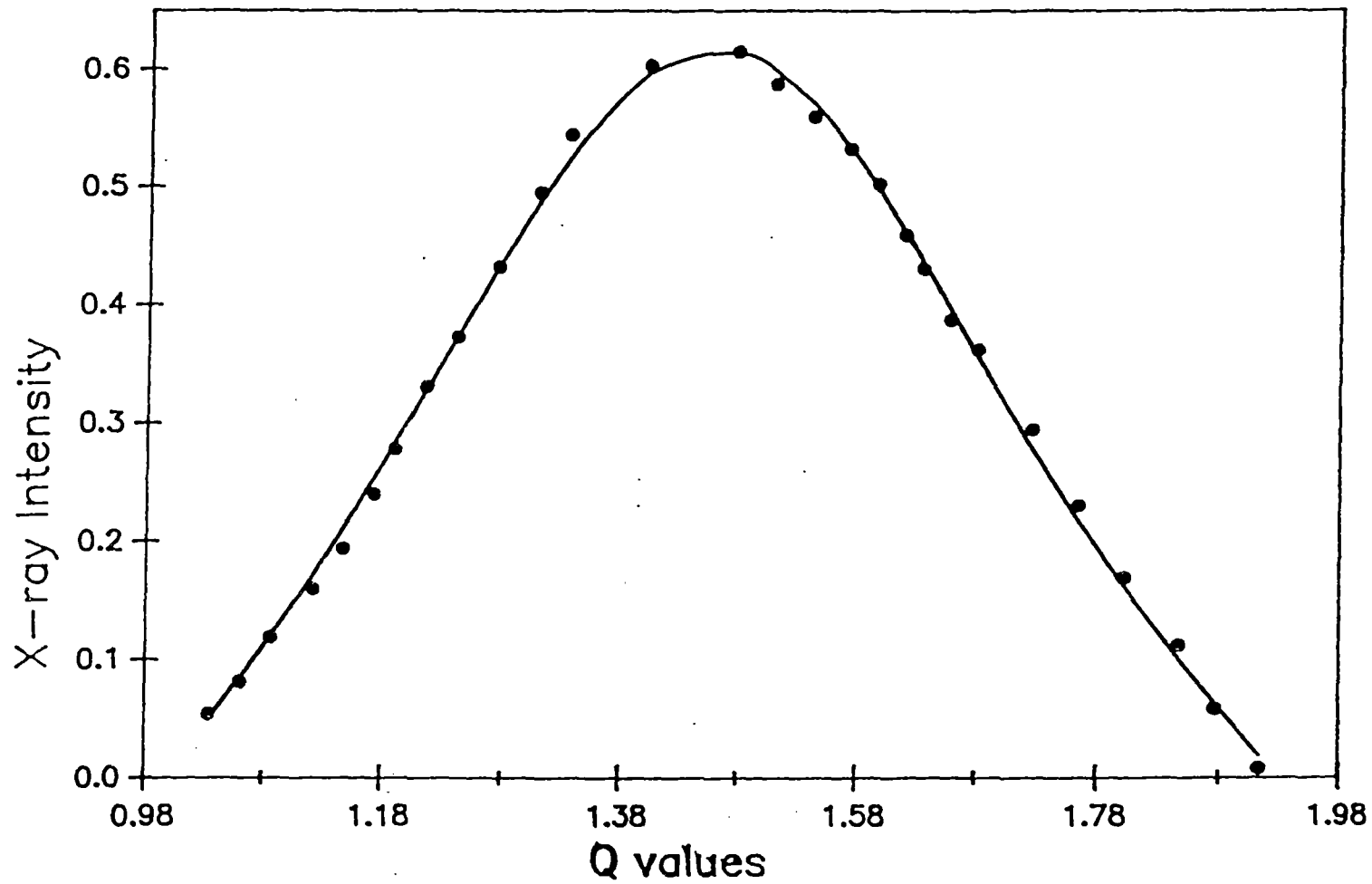
Figure 6.11 : Q vs intensity graph of sample 1d(3)CC at 50°C, o experimental points, —— fitted curve through calculated values.

molecules have dipole – dipole interaction forming dimers. The length (L), of the compound 1d(1)CC, measured from stereo-model unit was found to be 13.8 Å. I could not determine the pseudo layer spacing from x-ray diffraction photographs in the nematic phase. Probably this polar cyano compound also form dimers in the mesomorphic state, resulting in an increase in apparent value of l. Compound 1d(3)CCO2 is weakly polar and the layer spacing is found to be almost same as the molecular length (17.0 Å). Vander Waals type of interactions are involved in mesophase stability in this compound.

The compound 1d(3)CC exhibits a monotropic SmA phase with two collinear but incommensurate density modulation of periodicity 14.94Å which is almost the same as the molecular length and the other periodicity is 24.01Å, which is between l and 2l. This type of SmA phase is never been observed so far for pure compounds. We could not explain the existence of this smectic phase from the structural studies in the solid phase. Different kind of intermolecular interaction are responsible for this phase formation.

6.3.3 Orientational order parameters :

The mean intensity values of the four quardrants are given in tables 6.17 – 6.19 for the three compounds. The procedure for the determination of normalised orientational distribution function $f(\beta)$ values using Leadbetter's formula were described in chapter 5. Tables 6.20 – 6.22 give the normalised distribution function $f(\beta)$ values at angles of $5°$ intervals, calculated by an even power series of $\cos\beta$. Appearance of some negative values are due to the truncation errors. $f(\beta)$ versus β at different temperature are given in figures 6.12 – 6.14. The $\langle P_2 \rangle$ and $\langle P_4 \rangle$ values for the three compounds calculated from distribution function at different temperature are listed in table 6.23. Variation of $\langle P_2 \rangle$ and $\langle P_4 \rangle$ with temperatures are shown in figures 6.15 – 6.17.
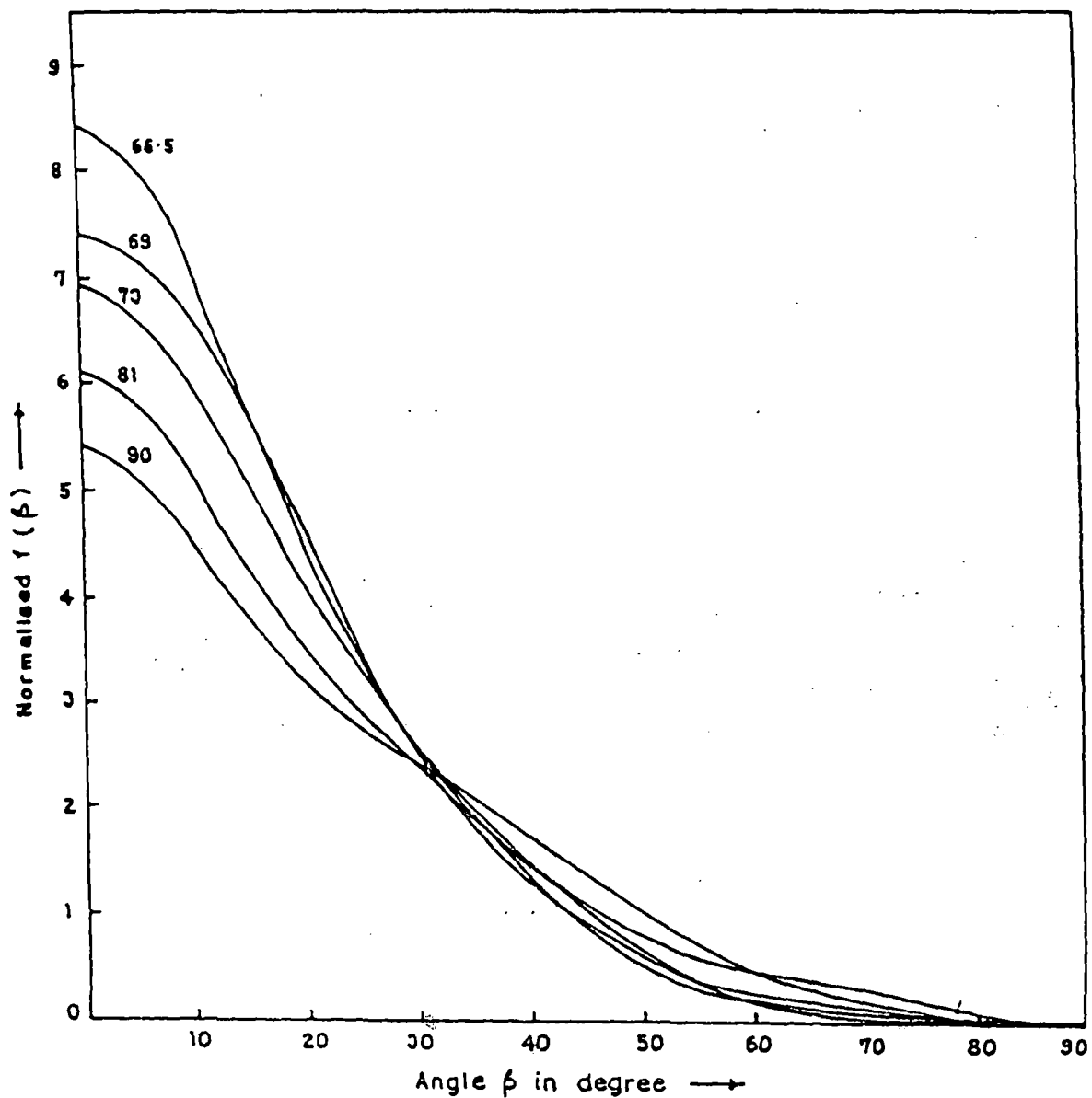
Figure 6.12 : Normalised orientational distribution function $f(\beta)$ plotted against the angle β at different temperatures of the sample 1d(1)CC.
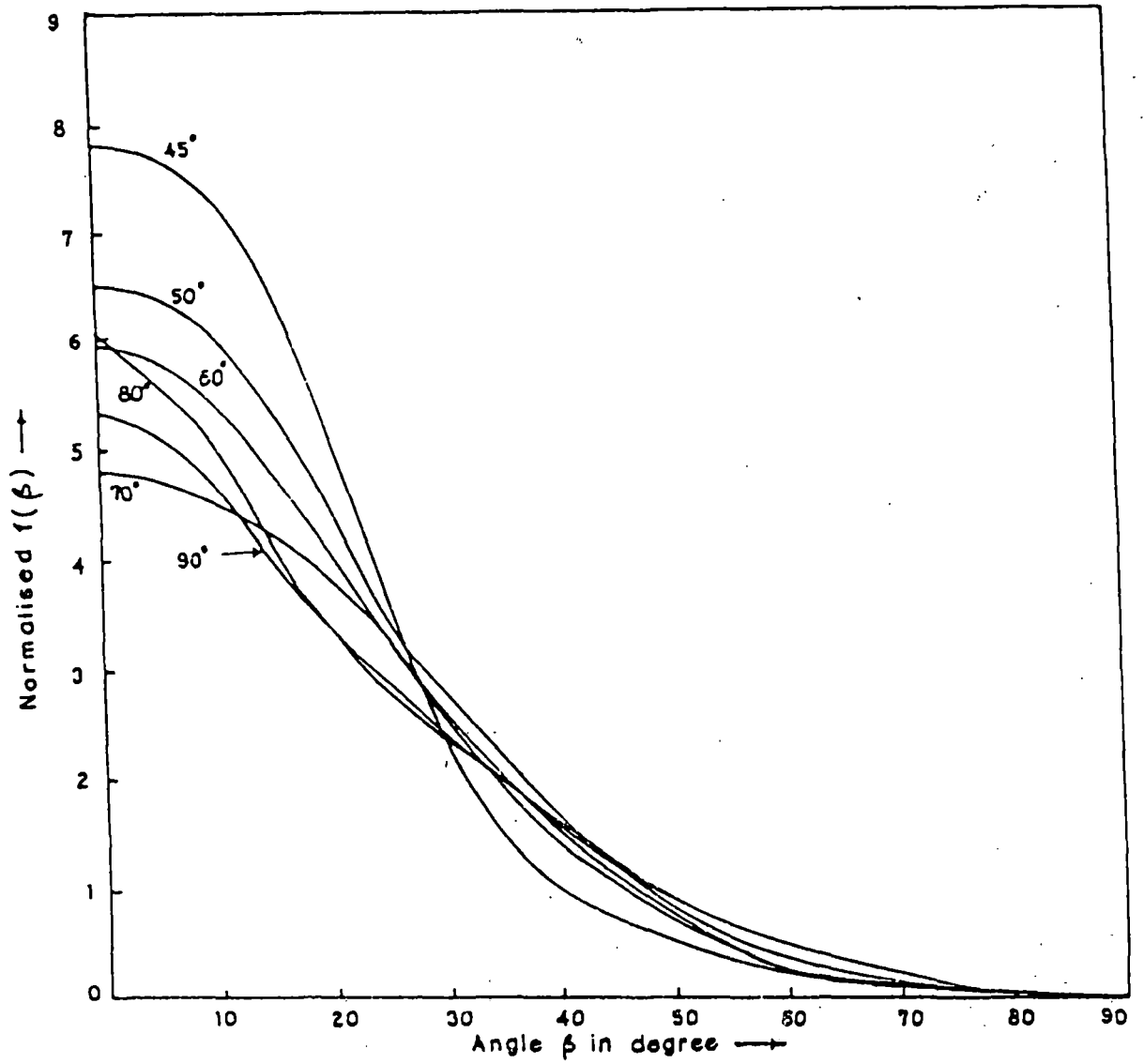
Figure 6.13 : Normalised orientational distribution function $f(\beta)$ plotted against the angle β at different temperatures of the sample 1d(3)CC.
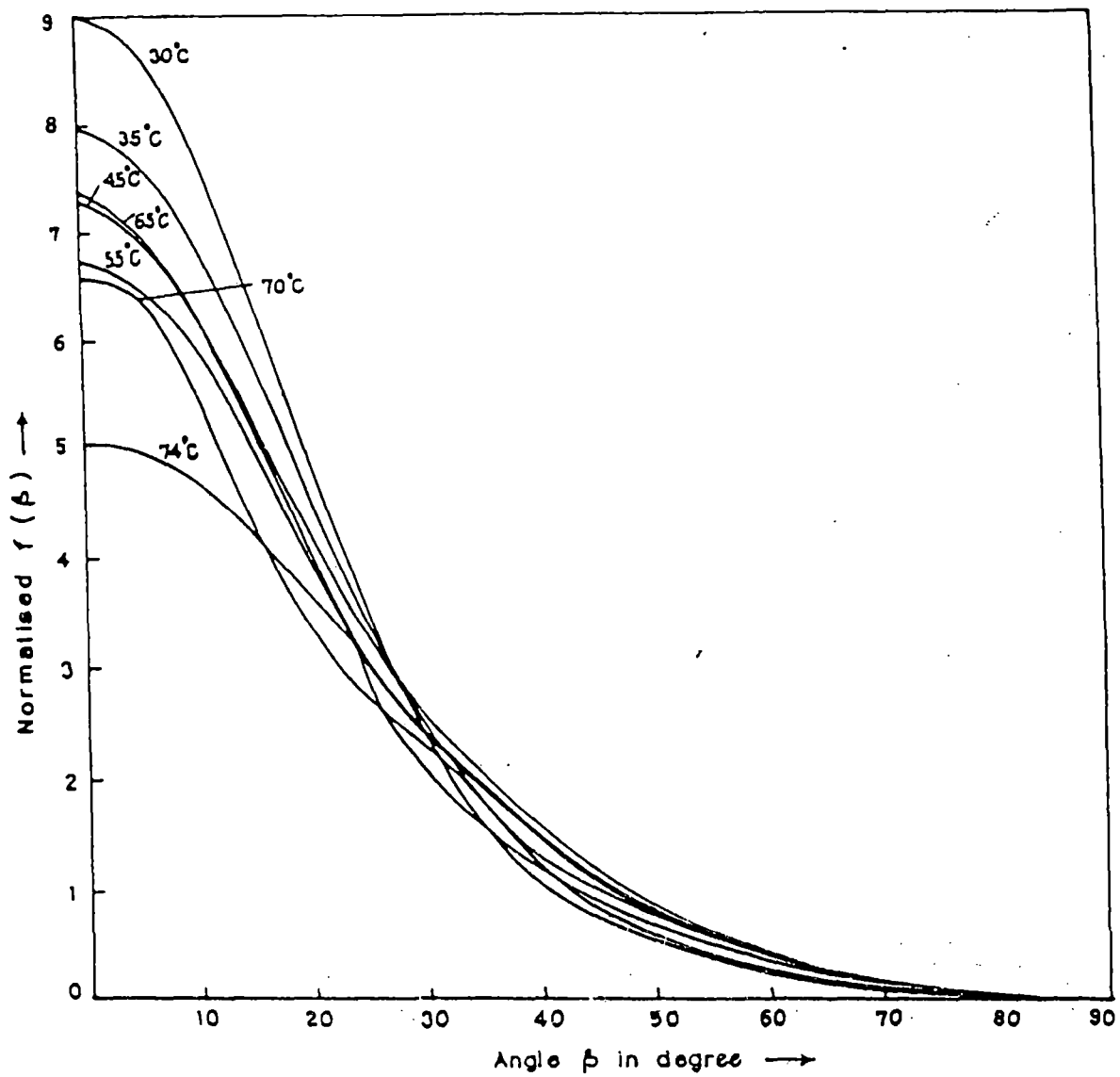
Figure 6.14 : Normalised orientational distribution function
$f(\beta)$ plotted against the angle β at different
temperatures of the sample 1d(3)CCO2.
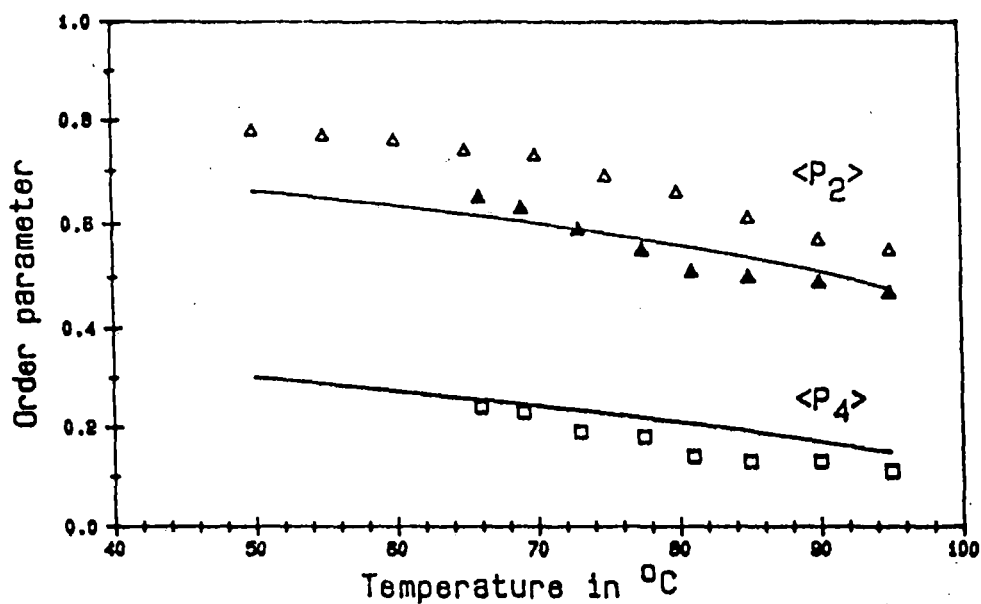
Figure 6.15 : Variation of order parameters $\langle P_2 \rangle$ and $\langle P_4 \rangle$
with temperature for the compound 1d(1)CC.

 - optical data,   - x-ray $\langle P_2 \rangle$ data

□ - x-ray $\langle P_4 \rangle$ data, —— MS theoretical values.
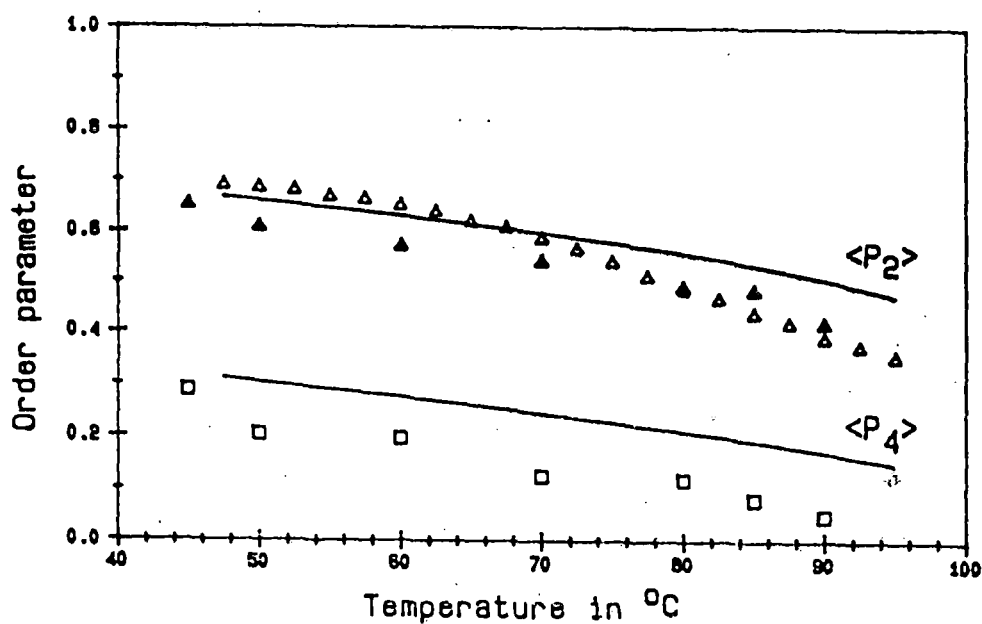
Figure 6.16 : Variation of order parameters $\langle P_2 \rangle$ and $\langle P_4 \rangle$
with temperature for the compound 1d(3)CC.

 - optical data,   - x-ray $\langle P_2 \rangle$ data

□ - x-ray $\langle P_4 \rangle$ data, —— MS theoretical values
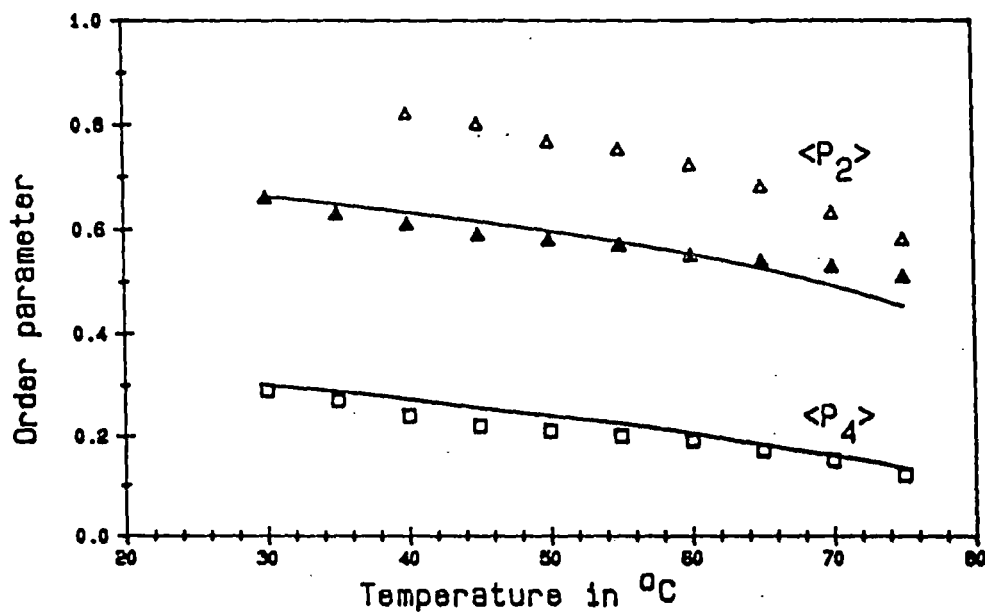
Figure 6.17 : Variation of order parameters $\langle P_2 \rangle$ and $\langle P_4 \rangle$ with temperature for the compound 1d(3)CCO2.

▲ - optical data, △ - x-ray $\langle P_2 \rangle$ data

□ - x-ray $\langle P_4 \rangle$ data, —— MS theoretical values

Some peculiarity was observed in the behaviour of 1d(1)CC. I could find supercooling in texture and birefringence study whereas in case of x-ray diffraction study no supercooling was observed. So order papameters from x-ray diffraction study could not be calculated for this particualr compound in the supercooled region.

The experimental uncertainties in both $\langle P_2 \rangle$ and $\langle P_4 \rangle$ are estimated to be ± 0.02. The order parameters $\langle P_2 \rangle$ and $\langle P_4 \rangle$ determined from x-ray data agree reasonably well with the MS theoretical curve for 1d(1)CC and 1d(3)CCO2. For the compound 1d(3)CC the $\langle P_2 \rangle$ values are in agreement whereas the $\langle P_4 \rangle$ values are less than calculated values. $\langle P_2 \rangle$ values determined from birefringence measurements for the compound 1d(3)CC are in good agreement with the theories apart from the fluctuations at high temperatures[14,15].

Surface treatment produced highly ordered molecules for compounds 1d(1)CC and 1d(3)CCO2, resulting in high value of order parameters determined by optical studies. The anisotropy of the alkenyl compound depends on the position of the double bond, the distance of the double bond from the core, the molecular structure and the specific steric conformation of the side chains. More studies on the physical properties of this type of alkenyl compounds are needed to give a quantitative explanation of the large discripancy between MS theoretical values and the experimental values.

TABLE − 6.1

Density (ρ) and refractive indices (n_o, n_e) at different temperatures of compound − 1d(1)CC.

Temp. in ^{o}C	Density(ρ) in gm/cm^3	$\lambda = 6907$ Å		$\lambda = 5780$ Å		$\lambda = 5461$ Å	
		n_o	n_e	n_o	n_e	n_o	n_e
50.0	1.114	1.418	1.511	1.421	1.513	1.426	1.519
52.5	1.112	1.418	1.510	1.421	1.513	1.426	1.518
55.0	1.110	1.418	1.509	1.421	1.512	1.426	1.517
57.5	1.108	1.418	1.509	1.421	1.511	1.426	1.516
60.0	1.107	1.418	1.508	1.421	1.510	1.426	1.516
62.5	1.105	1.418	1.507	1.421	1.509	1.426	1.515
65.0	1.104	1.418	1.506	1.421	1.508	1.426	1.514
67.5	1.102	1.418	1.504	1.421	1.507	1.426	1.512
70.0	1.100	1.418	1.503	1.421	1.506	1.426	1.511
72.5	1.099	1.418	1.502	1.421	1.504	1.426	1.509
75.0	1.097	1.419	1.500	1.422	1.502	1.426	1.508
77.5	1.095	1.419	1.498	1.422	1.500	1.426	1.506
80.0	1.093	1.420	1.496	1.423	1.499	1.427	1.504
82.5	1.091	1.421	1.495	1.424	1.497	1.428	1.502
85.0	1.089	1.422	1.493	1.424	1.495	1.429	1.501
87.5	1.087	1.422	1.492	1.425	1.494	1.430	1.499
90.0	1.085	1.423	1.490	1.426	1.492	1.431	1.497
92.5	1.083	1.423	1.489	1.426	1.491	1.432	1.496
95.0	1.080	1.424	1.487	1.426	1.489	1.432	1.494
100(iso)	1.072	1.428	1.428	1.431	1.431	1.436	1.436
102.5	1.062	1.428	1.428	1.431	1.431	1.436	1.436

TABLE - 6.2

Density (ρ) and refractive indices (n_o, n_e) at different temperatures of compound - 1d(3)CC.

Temp. in ^{o}C	Density(ρ) in gm/cm^3	λ = 6907 Å		λ = 5780 Å		λ = 5461 Å	
		n_o	n_e	n_o	n_e	n_o	n_e
47.5	1.138	1.408	1.515	1.411	1.518	1.417	1.524
50.0	1.136	1.408	1.514	1.411	1.517	1.417	1.524
52.5	1.133	1.408	1.513	1.411	1.516	1.417	1.522
55.0	1.131	1.408	1.512	1.411	1.514	1.417	1.521
57.5	1.128	1.408	1.510	1.411	1.513	1.417	1.519
60.0	1.126	1.408	1.508	1.411	1.511	1.417	1.517
62.5	1.124	1.408	1.506	1.411	1.509	1.417	1.515
65.0	1.121	1.408	1.504	1.411	1.506	1.417	1.513
67.5	1.119	1.408	1.501	1.411	1.504	1.417	1.510
70.0	1.117	1.409	1.498	1.412	1.501	1.418	1.507
72.5	1.115	1.409	1.495	1.412	1.498	1.418	1.504
75.0	1.113	1.410	1.492	1.413	1.495	1.419	1.501
77.5	1.110	1.411	1.489	1.414	1.491	1.419	1.498
80.0	1.108	1.412	1.486	1.415	1.488	1.420	1.495
82.5	1.105	1.413	1.483	1.416	1.486	1.421	1.492
85.0	1.102	1.414	1.480	1.417	1.483	1.422	1.489
87.5	1.099	1.415	1.478	1.418	1.481	1.424	1.487
90.0	1.097	1.416	1.475	1.420	1.478	1.425	1.484
92.5	1.094	1.417	1.473	1.420	1.476	1.426	1.481
95.0	1.092	1.417	1.470	1.420	1.473	1.426	1.479
100(iso)	1.082	1.423	1.423	1.426	1.426	1.432	1.432

TABLE - 6.3

Density (ρ) and refractive indices (n_o, n_e) at different temperatures of compound - 1d(3)CCO2.

Temp. in ^{o}C	Density(ρ) in gm/cm^3	λ = 6907 Å		λ = 5780 Å		λ = 5461 Å	
		n_o	n_e	n_o	n_e	n_o	n_e
37.5	1.035	1.387	1.500	1.391	1.502	1.398	1.510
40.0	1.033	1.387	1.499	1.391	1.501	1.398	1.509
42.5	1.031	1.387	1.497	1.391	1.500	1.398	1.507
45.0	1.029	1.387	1.495	1.391	1.498	1.398	1.505
47.5	1.027	1.387	1.494	1.391	1.496	1.398	1.503
50.0	1.024	1.387	1.492	1.391	1.494	1.398	1.502
52.5	1.022.	1.387	1.489	1.391	1.493	1.398	1.500
55.0	1.019	1.387	1.487	1.391	1.490	1.398	1.497
57.5	1.017	1.387	1.485	1.391	1.488	1.398	1.495
60.0	1.015	1.387	1.483	1.391	1.486	1.398	1.493
62.5	1.012	1.387	1.480	1.392	1.483	1.398	1.490
65.0	1.009	1.387	1.478	1.392	1.481	1.398	1.488
67.5	1.007	1.388	1.476	1.393	1.479	1.400	1.486
70.0	1.004	1.390	1.474	1.394	1.477	1.401	1.483
72.5	1.001	1.392	1.471	1.396	1.474	1.403	1.481
75.0	0.998	1.394	1.469	1.397	1.472	1.405	1.478
80.0	0.988	1.401	1.401	1.404	1.404	1.410	1.410

TABLE - 6.4

Polarizabilities (α_o, α_e) at different temperatures of compound - 1d(1)CC by Vuks' method.

Temp. in °C	$\lambda = 6907$ Å		$\lambda = 5780$ Å		$\lambda = 5461$ Å	
	α_o	α_e	α_o	α_e	α_o	α_e
50.0	20.29	25.73	20.42	25.83	20.63	26.07
52.5	20.33	25.75	20.46	25.85	20.67	26.09
55.0	20.37	25.74	20.50	25.87	20.71	26.08
57.5	20.41	25.76	20.54	25.86	20.75	26.10
60.0	20.43	25.73	20.56	25.83	20.77	26.07
62.5	20.47	25.72	20.61	25.82	20.82	26.08
65.0	20.51	25.70	20.64	25.80	20.85	26.04
67.5	20.54	25.65	20.67	25.78	20.89	25.99
70.0	20.59	25.64	20.72	25.74	20.93	25.96
72.5	20.61	25.58	20.74	25.68	20.96	25.90
75.0	20.68	25.54	20.82	25.62	21.00	25.86
77.5	20.75	25.47	20.89	25.55	21.06	25.83
80.0	20.83	25.40	20.98	25.53	21.14	25.76
82.5	20.92	25.38	21.05	25.46	21.23	25.68
85.0	21.01	25.31	21.13	25.39	21.33	25.63
87.5	21.10	25.26	21.22	25.34	20.12	25.90
90.0	21.18	25.21	21.32	25.29	21.54	25.51
92.5	21.24	25.18	21.36	25.25	21.61	25.47
95.0	21.32	25.16	21.43	25.24	21.70	25.45
100(iso)	22.01	22.01	22.14	22.14	22.35	22.35

TABLE - 6.5

Polarizabilities (α_o, α_e) at different temperatures of compound -1d(3)CC by Vuks' method.

Temp. in °C	$\lambda = 6907$ Å		$\lambda = 5780$ Å		$\lambda = 5461$ Å	
	α_o	α_e	α_o	α_e	α_o	α_e
47.5	21.72	28.64	21.86	28.78	22.14	29.06
50.0	21.77	28.63	21.91	28.77	22.18	29.08
52.5	21.83	28.64	21.97	28.78	22.25	29.06
55.0	21.87	28.63	22.02	28.71	22.30	29.06
57.5	21.94	28.59	22.08	28.73	23.38	28.89
60.0	21.99	28.52	22.13	28.66	23.42	28.94
62.5	22.04	28.45	22.18	28.59	23.47	28.87
65.0	22.11	28.40	22.26	28.49	23.54	28.83
67.5	22.17	28.27	22.31	28.41	23.60	28.70
70.0	22.25	28.13	22.39	28.28	22.68	28.56
72.5	22.33	27.99	22.48	28.14	22.76	28.42
75.0	22.44	27.85	22.59	27.99	22.85	28.29
77.5	22.57	27.73	22.70	27.82	22.95	28.17
80.0	22.66	27.59	22.81	27.67	23.07	28.03
82.5	22.79	25.47	22.94	27.61	23.20	27.91
85.0	22.92	27.34	23.10	27.48	23.33	27.79
87.5	23.08	27.28	23.23	27.42	23.52	27.71
90.0	23.19	27.13	23.37	27.27	23.63	27.57
92.5	23.32	27.07	23.47	27.21	23.77	27.45
95.0	23.38	26.93	23.53	27.08	23.82	27.37
100(iso)	24.38	24.38	24.53	24.53	24.82	24.82

TABLE - 6.6

Polarizabilities (α_o, α_e) at different temperatures of compound - 1d(3)CCO2 by Vuks' method.

Temp. in °C	$\lambda = 6907\ \overset{o}{A}$		$\lambda = 5780\ \overset{o}{A}$		$\lambda = 5461\ \overset{o}{A}$	
	α_o	α_e	α_o	α_e	α_o	α_e
37.5	24.43	33.06	24.67	33.14	25.05	33.60
40.0	24.48	33.05	24.72	33.13	25.11	33.56
42.5	24.54	32.97	24.78	33.09	25.17	33.52
45.0	24.61	32.91	24.85	33.06	25.24	33.45
47.5	24.67	32.86	24.91	32.98	25.30	33.38
50.0	24.74	32.80	24.98	32.92	25.37	33.35
52.5	24.81	32.69	25.04	32.88	25.43	33.27
55.0	24.89	32.64	25.13	32.79	25.53	33.19
57.5	24.95	32.56	25.19	32.71	25.59	33.11
60.0	25.03	32.49	25.26	32.65	25.67	33.01
62.5	25.11	32.36	25.38	32.51	25.75	32.91
65.0	25.20	32.31	25.50	32.45	25.84	32.87
67.5	25.32	32.21	25.59	32.36	26.00	32.73
70.0	25.54	32.13	25.78	32.25	26.19	32.62
72.5	25.73	31.99	25.97	32.14	26.41	32.54
75.0	25.95	31.91	26.16	32.07	26.64	32.39
80.0(Iso)	27.14	27.14	27.32	27.32	27.68	27.68

TABLE - 6.7

Polarizabilities (α_o, α_e) at different temperatures of compound - 1d(1)CC by Neugebauer's method.

Temp. in °C	$\lambda = 6907 \text{ Å}$		$\lambda = 5780 \text{ Å}$		$\lambda = 5461 \text{ Å}$	
	α_o	α_e	α_o	α_e	α_o	α_e
50.0	20.56	25.19	20.69	25.29	20.90	25.52
52.5	20.60	25.21	20.73	25.31	20.94	26.54
55.0	20.63	25.21	20.76	25.33	20.98	26.54
57.5	20.67	25.23	20.80	25.33	20.02	26.56
60.0	20.69	25.20	20.82	25.31	20.04	26.54
62.5	20.73	25.20	20.86	25.30	20.08	26.55
65.0	20.76	25.19	20.89	25.29	20.11	26.52
67.5	20.79	25.15	20.92	25.27	21.14	25.48
70.0	20.83	25.15	20.97	25.25	20.18	25.46
72.5	20.85	25.10	20.99	25.20	20.21	25.41
75.0	20.92	25.06	20.05	25.14	21.25	25.38
77.5	20.98	25.01	21.12	25.09	21.30	25.35
80.0	21.05	24.95	21.20	25.08	21.37	25.30
82.5	21.14	24.94	21.27	25.02	21.45	25.24
85.0	21.22	24.89	21.34	24.97	21.54	25.21
87.5	21.30	24.85	21.42	24.93	20.40	25.35
90.0	21.38	24.82	21.51	24.90	21.73	25.11
92.5	21.43	24.79	21.56	24.87	21.80	25.08
95.0	21.51	24.78	21.62	24.87	21.89	25.08
100(iso)	22.01	22.01	22.14	22.14	22.35	22.35

TABLE - 6.8

Polarizabilities (α_o, α_e) at different temperatures of compound - 1d(3)CC by Neugebauer's method.

Temp. in °C	$\lambda = 6907$ Å		$\lambda = 5780$ Å		$\lambda = 5461$ Å	
	α_o	α_e	α_o	α_e	α_o	α_e
47.5	22.06	27.96	22.20	28.10	22.49	28.37
50.0	22.10	27.96	22.24	28.09	22.53	28.39
52.5	22.16	27.98	22.31	28.11	22.59	28.39
55.0	22.20	27.97	22.35	28.06	22.63	28.38
57.5	22.27	27.94	22.41	28.08	22.70	28.25
60.0	22.31	27.88	22.45	28.02	22.74	28.30
62.5	22.35	27.83	22.50	27.96	22.79	28.24
65.0	22.42	27.79	22.56	27.88	22.85	28.21
67.5	22.46	27.68	22.61	27.82	22.90	28.10
70.0	22.53	27.57	22.68	27.71	22.97	27.98
72.5	22.61	27.45	22.75	27.59	23.04	27.87
75.0	22.70	27.33	22.85	27.47	23.12	27.75
77.5	22.82	27.23	22.95	27.32	23.21	27.66
80.0	22.90	27.12	23.04	27.20	23.31	27.54
82.5	23.01	27.02	23.16	27.16	23.43	27.45
85.0	23.14	26.92	23.31	27.06	23.55	27.35
87.5	23.28	26.88	23.43	27.02	23.72	27.31
90.0	23.38	26.75	23.55	26.89	23.82	27.19
92.5	23.50	26.71	23.65	26.86	23.95	27.09
95.0	23.55	26.59	23.70	26.74	24.00	27.03
100(iso)	24.38	24.38	24.53	24.53	24.82	24.82

TABLE - 6.9

Polarizabilities (α_o, α_e) at different temperatures of compound - 1d(3)CCO2 by Neugebauer's method.

Temp. in °C	$\lambda = 6907 \overset{o}{A}$		$\lambda = 5780 \overset{o}{A}$		$\lambda = 5461 \overset{o}{A}$	
	α_o	α_e	α_o	α_e	α_o	α_e
37.5	24.84	32.25	25.07	32.34	25.46	32.78
40.0	24.89	32.24	25.12	32.34	25.51	32.75
42.5	24.94	32.18	25.17	32.30	25.57	32.71
45.0	25.00	32.13	25.23	32.29	25.63	32.67
47.5	25.05	32.10	25.29	32.22	25.69	32.60
50.0	25.12	32.05	25.35	32.17	25.75	32.59
52.5	25.17	31.95	25.41	32.14	25.81	32.52
55.0	25.25	31.92	25.49	32.07	25.89	32.46
57.5	25.31	31.85	25.54	32.01	25.95	32.40
60.0	25.37	31.80	25.61	31.96	26.02	32.32
62.5	25.44	31.69	25.71	31.84	26.09	32.24
65.0	25.52	31.65	25.82	31.80	26.17	32.20
67.5	25.64	31.57	25.91	31.73	26.32	32.09
70.0	25.84	31.52	26.08	31.65	26.49	32.01
72.5	26.02	31.41	26.26	31.57	26.70	31.96
75.0	26.23	31.36	26.43	31.52	26.91	31.85
80.0(Iso)	27.14	27.14	27.32	27.32	27.68	27.68

TABLE - 6.10

Order parameter $\langle P_2 \rangle$ of compound - 1d(1)CC at different temperature by Vuks' method.

$(\alpha_{\parallel} - \alpha_{\perp}) = 6.89$ in 10^{-24} cm^3 unit.

Temp. in °C	$\lambda = 6907$ Å	$\lambda = 5780$ Å	$\lambda = 5461$ Å	Average
	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$
50.0	0.7817	0.7852	0.7896	0.7855
52.5	0.7788	0.7823	0.7866	0.7826
55.0	0.7717	0.7793	0.7794	0.7768
57.5	0.7688	0.7721	0.7765	0.7725
60.0	0.7602	0.7634	0.7678	0.7638
62.5	0.7529	0.7562	0.7634	0.7575
65.0	0.7458	0.7489	0.7533	0.7493
67.5	0.7343	0.7417	0.7417	0.7392
70.0	0.7271	0.7300	0.7300	0.7290
72.5	0.7142	0.7170	0.7170	0.7161
75.0	0.6983	0.6967	0.7054	0.7001
77.5	0.6783	0.6763	0.6923	0.6823
80.0	0.6581	0.6604	0.6705	0.6620
82.5	0.6409	0.6386	0.6459	0.6418
85.0	0.6165	0.6183	0.6241	0.6196
87.5	0.5978	0.5980	0.5951	0.5969
90.0	0.5791	0.5762	0.5762	0.5772
92.5	0.5662	0.5646	0.5602	0.5636
95.0	0.5518	0.5530	0.5443	0.5497

TABLE - 6.11

Order parameter $\langle P_2 \rangle$ of compound - 1d(3)CC at different temperature by Vuks' method.

$(\alpha_\parallel - \alpha_\perp) = 9.924$ in 10^{-24} cm^3 unit.

Temp. in $^{\circ}C$	$\lambda = 6907 \ \overset{\circ}{A}$	$\lambda = 5780 \ \overset{\circ}{A}$	$\lambda = 5461 \ \overset{\circ}{A}$	Average
	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$
47.5	0.7076	0.6963	0.6997	0.7012
50.0	0.7014	0.6913	0.6977	0.6968
52.5	0.6963	0.6862	0.6896	0.6907
55.0	0.6912	0.6741	0.6845	0.6832
57.5	0.6799	0.6701	0.6592	0.6697
60.0	0.6677	0.6580	0.6613	0.6623
62.5	0.6554	0.6459	0.6491	0.6501
65.0	0.6431	0.6278	0.6369	0.6359
67.5	0.6237	0.6146	0.6177	0.6186
70.0	0.6012	0.5925	0.5954	0.5964
72.5	0.5787	0.5703	0.5732	0.5741
75.0	0.5532	0.5441	0.5508	0.5494
77.5	0.5266	0.5159	0.5286	0.5237
80.0	0.5041	0.4897	0.5023	0.4990
82.5	0.4785	0.4705	0.4769	0.4753
85.0	0.4519	0.4423	0.4506	0.4483
87.5	0.4294	0.4232	0.4253	0.4259
90.0	0.4029	0.3929	0.3989	0.3982
92.5	0.3824	0.3768	0.3726	0.3772
95.0	0.3629	0.3577	0.3595	0.3600

TABLE - 6.12

Order parameter $\langle P_2 \rangle$ of compound - 1d(3)CCO2 at different temperature by Vuks' method.

$(\alpha_{\parallel} - \alpha_{\perp}) = 9.974$ in 10^{-24} cm^3 unit.

Temp. in °C	$\lambda = 6907$ Å	$\lambda = 5780$ Å	$\lambda = 5461$ Å	Average
	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$
37.5	0.8566	0.8492	0.8572	0.8543
40.0	0.8507	0.8432	0.8472	0.8470
42.5	0.8368	0.8332	0.8372	0.8357
45.0	0.8229	0.8241	0.8231	0.8233
47.5	0.8130	0.8101	0.8101	0.8111
50.0	0.8001	0.7961	0.8001	0.7987
52.5	0.7822	0.7860	0.7860	0.7847
55.0	0.7683	0.7690	0.7690	0.7687
57.5	0.7544	0.7539	0.7540	0.7541
60.0	0.7405	0.7409	0.7369	0.7394
62.5	0.7197	0.7148	0.7189	0.7178
65.0	0.7057	0.6968	0.7048	0.7024
67.5	0.6839	0.6787	0.6748	0.6791
70.0	0.6542	0.6486	0.6447	0.6491
72.5	0.6204	0.6186	0.6146	0.6178
75.0	0.5906	0.5925	0.5775	0.5868

TABLE - 6.13

Order parameter $\langle P_2 \rangle$ of compound - 1d(1)CC at different temperature by Neugebauer's method.

$(\alpha_{\parallel} - \alpha_{\perp}) = 5.812$ in 10^{-24} cm^3 unit.

Temp. in °C	$\lambda = 6907 \overset{\circ}{A}$	$\lambda = 5780 \overset{\circ}{A}$	$\lambda = 5461 \overset{\circ}{A}$	Average
	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$	$\langle P_2 \rangle$
50.0	0.7966	0.7915	0.7908	0.7929
52.5	0.7849	0.7897	0.7874	0.7873
55.0	0.7863	0.7863	0.7806	0.7844
57.5	0.7846	0.7794	0.7771	0.7804
60.0	0.7760	0.7708	0.7703	0.7723
62.5	0.7691	0.7639	0.7652	0.7661
65.0	0.7605	0.7553	0.7549	0.7569
67.5	0.7502	0.7485	0.7429	0.7472
70.0	0.7416	0.7364	0.7309	0.7363
72.5	0.7295	0.7244	0.7189	0.7242
75.0	0.7140	0.7037	0.7069	0.7082
77.5	0.6934	0.6831	0.6950	0.6905
80.0	0.6727	0.6676	0.6727	0.6710
82.5	0.6555	0.6452	0.6488	0.6498
85.0	0.6297	0.6245	0.6265	0.6269
87.5	0.6108	0.6039	0.5991	0.6046
90.0	0.5919	0.5833	0.5786	0.5846
92.5	0.5781	0.5712	0.5632	0.5708
95.0	0.5643	0.5592	0.5460	0.5565

TABLE - 6.14

Order parameter $\langle P_2 \rangle$ of compound - 1d(3)CC at different temperature by Neugebauer's method.

$(\alpha_{\parallel} - \alpha_{\perp}) = 8.499$ in 10^{-24} cm^3 unit.

Temp. in $^{\circ}C$	$\lambda = 6907\ \AA$ $\langle P_2 \rangle$	$\lambda = 5780\ \AA$ $\langle P_2 \rangle$	$\lambda = 5461\ \AA$ $\langle P_2 \rangle$	Average $\langle P_2 \rangle$
47.5	0.7011	0.6930	0.7058	0.6999
50.0	0.6964	0.6883	0.7034	0.6960
52.5	0.6916	0.6836	0.6962	0.6905
55.0	0.6856	0.6718	0.6902	0.6825
57.5	0.6749	0.6671	0.6662	0.6694
60.0	0.6619	0.6553	0.6674	0.6615
62.5	0.6500	0.6436	0.6542	0.6492
65.0	0.6393	0.6247	0.6434	0.6358
67.5	0.6203	0.6130	0.6242	0.6192
70.0	0.5977	0.5918	0.6014	0.5969
72.5	0.5752	0.5694	0.5797	0.5747
75.0	0.5502	0.5436	0.5569	0.5502
77.5	0.5240	0.5153	0.5341	0.5244
80.0	0.5015	0.4894	0.5077	0.4995
82.5	0.4753	0.4706	0.4825	0.4761
85.0	0.4504	0.4412	0.4561	0.4492
87.5	0.4278	0.4224	0.4297	0.4266
90.0	0.4005	0.3929	0.4033	0.3989
92.5	0.3815	0.3776	0.3769	0.3786
95.0	0.3613	0.3576	0.3637	0.3608

TABLE – 6.15

Order parameter $\langle P_2 \rangle$ of compound – 1d(3)CCO2 at different temperature by Neugebauer's method.

$(\alpha_\parallel - \alpha_\perp) = 8.758$ in 10^{-24} cm^3 unit.

Temp. in °C	$\lambda = 6907$ Å $\langle P_2 \rangle$	$\lambda = 5780$ Å $\langle P_2 \rangle$	$\lambda = 5461$ Å $\langle P_2 \rangle$	Average $\langle P_2 \rangle$
37.5	0.8631	0.8301	0.8686	0.8539
40.0	0.8573	0.8244	0.8592	0.8469
42.5	0.8433	0.8141	0.8497	0.8357
45.0	0.8305	0.8050	0.8354	0.8236
47.5	0.8200	0.7913	0.8223	0.8112
50.0	0.8072	0.7787	0.8116	0.7991
52.5	0.7897	0.7684	0.7986	0.7855
55.0	0.7758	0.7525	0.7807	0.7696
57.5	0.7618	0.7388	0.7665	0.7557
60.0	0.7490	0.7251	0.7487	0.7409
62.5	0.7268	0.6999	0.7308	0.7191
65.0	0.7140	0.6828	0.7178	0.7048
67.5	0.6919	0.6645	0.6868	0.6810
70.0	0.6616	0.6360	0.6559	0.6511
72.5	0.6278	0.6063	0.6262	0.6201
75.0	0.5975	0.5812	0.5870	0.5885

TABLE - 6.17

Mean experimental intensity values I(ψ), in arbitrary units, of compound - 1d(1)CC after background correction.

ψ (degree)	I(ψ) values at different temperatures in $^{\circ}$ C							
	66.5	69	73	77	81	85	90	95
0	37.5	36.0	37.5	29.0	22.0	34.0	37.0	30.0
5	36.0	35.0	36.5	28.5	20.5	33.5	35.5	29.0
10	32.0	32.0	34.0	26.0	19.0	31.0	32.5	27.0
15	27.0	28.0	29.0	23.0	17.0	27.0	30.0	25.0
20	23.0	23.0	25.0	19.5	15.0	23.0	26.5	22.0
25	18.0	18.5	21.0	16.5	13.0	18.0	24.0	19.0
30	14.0	14.0	17.0	13.0	10.5	14.0	21.0	16.0
35	10.0	9.5	13.0	10.5	9.0	10.5	18.0	13.0
40	7.5	8.5	10.0	8.5	7.0	8.0	14.5	11.0
45	5.0	5.5	7.0	6.0	5.5	6.0	11.5	9.0
50	3.5	4.0	5.0	5.0	4.5	5.0	10.5	7.5
55	2.5	2.5	3.5	4.0	3.5	4.0	6.5	6.0
60	1.5	1.5	2.2	3.0	3.0	3.0	4.5	5.0
65	1.2	1.0	1.5	2.0	2.0	2.0	3.0	3.5
70	1.0	0.8	1.0	1.8	1.5	1.5	2.0	3.0
75	0.8	0.5	0.8	1.0	1.0	1.0	1.0	2.0
80	0.5	0.3	0.5	0.5	0.5	0.5	0.5	1.5
85	0.2	0.1	0.1	0.2	0.2	0.2	0.1	1.0
90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

TABLE - 6.18

Mean experimental intensity values I(ψ), in arbitrary units, of compound - 1d(3)CC after background correction.

ψ (degree)	I(ψ) values at different temperatures in ^{o} C					
	45	50	60	70	80	90
0	73.0	67.0	70.0	58.5	35.0	39.0
5	71.0	66.0	69.0	58.0	33.5	38.0
10	65.0	63.0	65.0	56.0	31.0	35.0
15	57.0	55.0	58.0	51.0	28.0	32.0
20	46.0	46.0	50.0	46.5	24.0	29.0
25	32.0	37.0	42.0	40.0	20.5	25.0
30	23.0	29.0	34.0	34.0	18.0	21.0
35	16.0	23.0	26.5	26.5	15.5	18.0
40	12.0	17.0	21.0	20.0	12.3	15.0
45	9.0	12.0	15.5	15.0	9.5	11.0
50	7.0	8.0	11.0	11.0	7.5	9.0
55	5.0	6.0	8.0	7.5	6.0	7.0
60	4.0	4.0	5.5	5.0	4.5	5.0
65	2.0	2.0	4.0	4.0	3.0	4.0
70	1.5	1.0	2.0	2.5	1.8	2.5
75	1.0	0.5	1.5	1.5	1.0	1.5
80	0.0	0.0	0.5	1.0	0.5	1.0
85	0.0	0.0	0.0	0.0	0.0	0.0
90	0.0	0.0	0.0	0.0	0.0	0.0

TABLE - 6.19

Mean experimental intensity values $I(\psi)$, in arbitrary units, of compound - 1d(3)CCO2 after background correction.

ψ (degree)	$I(\psi)$ values at different temperatures in ^{o} C					
	30	35	40	45	50	55
0	65.0	53.2	43.0	44.0	47.0	54.5
5	63.0	51.5	42.0	43.0	46.0	53.0
10	56.0	47.5	38.0	39.5	43.0	49.0
15	46.5	40.0	33.0	34.0	38.0	42.5
20	38.0	33.0	28.0	28.0	32.0	36.0
25	28.0	26.0	22.0	23.0	26.5	30.0
30	20.0	20.0	16.5	18.0	21.0	24.0
35	14.5	14.0	11.5	14.0	16.0	19.5
40	11.0	10.0	8.5	10.0	13.0	16.0
45	8.0	7.5	6.5	8.0	9.5	12.0
50	6.0	5.5	5.0	6.5	7.0	9.0
55	4.0	4.0	4.0	5.0	5.0	6.0
60	2.5	2.5	3.0	3.0	3.5	4.0
65	1.5	2.0	2.5	2.5	2.0	2.5
70	1.0	1.0	1.5	1.5	1.0	1.5
75	0.5	0.8	1.0	1.0	0.5	1.0
80	0.2	0.5	0.5	0.5	0.2	0.5
85	0.1	0.2	0.2	0.0	0.1	0.2
90	0.0	0.0	0.0	0.0	0.0	0.0

TABLE – 6.19

Mean experimental intensity values $I(\psi)$, in arbitrary units, of compound – 1d(3)CCO2 after background correction.

ψ (degree)	$I(\psi)$ values at different temperatures in ℃			
	60	65	70	74
0	53.2	46.5	44.0	34.0
5	51.0	44.5	42.5	33.0
10	46.5	40.5	38.0	31.0
15	40.0	35.0	32.5	28.0
20	32.0	28.0	28.0	26.0
25	26.0	22.0	24.5	22.0
30	21.0	18.0	21.0	18.0
35	17.0	15.0	17.0	15.0
40	14.5	13.0	13.0	12.0
45	11.2	10.5	11.5	9.5
50	9.0	8.5	9.0	7.0
55	7.0	6.5	7.0	5.0
60	5.5	5.0	6.0	3.5
65	4.0	3.0	4.5	2.5
70	2.8	2.5	3.5	2.0
75	1.5	1.5	2.0	1.5
80	1.0	1.0	1.5	1.0
85	0.5	0.5	1.0	0.5
90	0.0	0.0	0.0	0.0

TABLE - 6.20

Normalised distribution function f(β) values at different temperatures of compound - 1d(1)CC.

β (degree)	f(β) values at temperatures in °C					
	66.5	69	73	77	81	85
0	8.42	7.39	6.93	6.46	6.06	6.72
5	8.03	7.19	6.66	6.23	5.79	6.55
10	7.01	6.61	5.95	5.61	5.09	6.06
15	5.69	5.71	5.01	4.77	4.25	5.29
20	4.42	4.60	4.08	3.89	3.48	4.37
25	3.37	3.48	3.27	3.10	2.89	3.38
30	2.55	2.52	2.60	2.42	2.40	2.48
35	1.88	1.79	2.02	1.86	1.94	1.74
40	1.31	1.29	1.49	1.39	1.49	1.21
45	0.85	0.93	1.05	1.02	1.10	0.86
50	0.52	0.63	0.69	0.74	0.81	0.65
55	0.32	0.40	0.44	0.55	0.63	0.51
60	0.22	0.23	0.29	0.42	0.51	0.39
65	0.16	0.14	0.19	0.32	0.39	0.29
70	0.12	0.09	0.12	0.22	0.27	0.19
75	0.07	0.05	0.07	0.14	0.16	0.11
80	0.04	0.03	0.04	0.06	0.07	0.05
85	0.02	0.01	0.01	0.02	0.02	0.02
90	0.01	0.003	0.008	0.005	0.01	0.01

(continued)

TABLE - 6.20

Normalised distribution function $f(\beta)$ values at different temperatures of compound - 1d(1)CC.

β (degree)	$f(\beta)$ values at temperatures in $^{\circ}$ C		
	90	95	
0	5.35	4.98	
5	5.12	4.85	
10	4.52	4.50	
15	3.80	3.99	
20	3.17	3.41	
25	2.72	2.83	
30	2.38	2.29	
35	2.05	1.83	
40	1.71	1.45	
45	1.35	1.13	
50	1.03	0.89	
55	0.77	0.71	
60	0.54	0.56	
65	0.35	0.44	
70	0.20	0.33	
75	0.09	0.22	
80	0.03	0.13	
85	0.01	0.06	
90	0.008	0.04	

TABLE - 6.21

Normalised distribution function f(β) values at different temperatures of compound - 1d(3)CC.

β (degree)	f(β) values at temperatures in °C					
	45	50	60	70	80	90
0	7.76	6.46	5.89	4.77	5.98	5.29
5	7.67	6.35	5.76	4.70	5.72	5.11
10	7.32	6.00	5.37	4.51	5.03	4.61
15	6.51	5.36	4.78	4.21	4.18	3.98
20	5.22	4.48	4.06	3.80	3.41	3.38
25	3.71	3.49	3.30	3.32	2.81	2.87
30	2.37	2.59	2.59	2.77	2.36	2.44
35	1.45	1.90	1.99	2.20	1.96	2.02
40	0.95	1.39	1.49	1.65	1.58	1.61
45	0.71	1.02	1.09	1.17	1.22	1.23
50	0.55	0.71	0.77	0.80	0.92	0.91
55	0.40	0.45	0.53	0.54	0.69	0.68
60	0.26	0.27	0.35	0.36	0.51	0.51
65	0.16	0.15	0.23	0.25	0.36	0.37
70	0.10	0.08	0.14	0.16	0.23	0.25
75	0.06	0.05	0.08	0.09	0.12	0.15
80	0.03	0.02	0.04	0.05	0.05	0.07
85	0.001	-0.002	0.006	0.01	0.00	0.02
90	-0.011	-0.010	-0.005	0.00	0.00	0.001

TABLE - 6.22

Normalised distribution function $f(\beta)$ values at different temperatures of compound - 1d(3)CCO2.

β (degree)	$f(\beta)$ values at temperatures in $^{\circ}$ C					
	30	35	40	45	50	55
0	9.081	7.979	7.399	7.263	6.457	6.724
5	8.729	7.690	7.124	6.997	6.288	6.496
10	7.756	6.902	6.374	6.277	5.807	5.862
15	6.372	5.806	5.344	5.288	5.082	4.964
20	4.857	4.618	4.256	4.236	4.219	3.988
25	3.464	3.503	3.278	3.267	3.337	3.099
30	2.357	2.547	2.482	2.447	2.541	2.393
35	1.578	1.780	1.860	1.788	1.892	1.871
40	1.077	1.203	1.374	1.284	1.400	1.475
45	0.760	0.802	0.988	0.921	1.036	1.141
50	0.544	0.543	0.684	0.674	0.758	0.836
55	0.377	0.382	0.456	0.505	0.536	0.567
60	0.244	0.271	0.297	0.376	0.354	0.356
65	0.144	0.182	0.191	0.262	0.212	0.213
70	0.075	0.110	0.121	0.163	0.112	0.125
75	0.035	0.057	0.072	0.086	0.050	0.072
80	0.014	0.026	0.036	0.036	0.018	0.036
85	0.006	0.013	0.013	0.011	0.004	0.012
90	0.004	0.010	0.005	0.004	0.001	0.004

(continued)

TABLE - 6.22

Normalised distribution function $f(\beta)$ values at different temperatures of compound - 1d(3)CCO2.

β (degree)	$f(\beta)$ values at temperatures in $^\circ$ C			
	60	65	70	74
0	7.431	7.347	6.858	5.095
5	7.124	7.069	6.468	4.983
10	6.286	6.290	5.483	4.664
15	5.135	5.165	4.320	4.188
20	3.935	3.929	3.353	3.627
25	2.903	2.829	2.703	3.054
30	2.139	2.027	2.262	2.519
35	1.630	1.542	1.869	2.039
40	1.289	1.272	1.459	1.606
45	1.029	1.079	1.079	1.216
50	0.803	0.877	0.798	0.877
55	0.604	0.659	0.628	0.607
60	0.442	0.462	0.520	0.415
65	0.319	0.314	0.418	0.289
70	0.224	0.213	0.303	0.203
75	0.143	0.138	0.188	0.136
80	0.074	0.076	0.099	0.079
85	0.024	0.031	0.047	0.038
90	0.006	0.013	0.003	0.023

TABLE - 6.23

Order parameter values at different temperatures of compounds - 1d(1)CC, 1d(3)CC and 1d(3)CCO2 from x-ray diffraction study.

sample - 1d(1)CC			sample - 1d(3)CC			sample - 1d(3)CCO2		
Temp. in $^{\circ}$C	$\langle P_2 \rangle$	$\langle P_4 \rangle$	Temp. in $^{\circ}$C	$\langle P_2 \rangle$	$\langle P_4 \rangle$	Temp. in $^{\circ}$C	$\langle P_2 \rangle$	$\langle P_4 \rangle$
66.5	0.65	0.25	45.0	0.66	0.29	30.0	0.66	0.29
69.0	0.63	0.23	50.0	0.61	0.20	35.0	0.63	0.27
73.0	0.59	0.19	60.0	0.57	0.19	40.0	0.61	0.24
77.0	0.55	0.18	70.0	0.55	0.12	45.0	0.59	0.22
81.0	0.51	0.14	80.0	0.49	0.11	50.0	0.58	0.21
85.0	0.50	0.13	85.0	0.48	0.08	55.0	0.57	0.20
90.0	0.49	0.12	90.0	0.42	0.05	60.0	0.55	0.19
95.0	0.47	0.11				65.0	0.54	0.17
						70.0	0.53	0.15
						74.0	0.52	0.12

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