Order Parameter Temperature Dependence of Some Nematic Liquids Related to Magnetic and Optical Anisotropies

I. H. Ibrahim and W. Haase

Institut für Physikalische Chemie, Technische Hochschule, Darmstadt

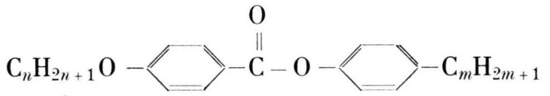
(Z. Naturforsch. **31 a,** 1644—1650 [1976]; received November 6, 1976)

The diamagnetic susceptibilities, refractive indices and densities were measured as a function of temperature for three 4,4′-disubstituted benzoic acid-phenylester compounds. The polarizabilities were calculated using the Vuks formula and Neugebauer's relations. The orientational order parameters obtained from the magnetic and from the optical data as a function of temperature, in the absence of single crystal data, were compared.

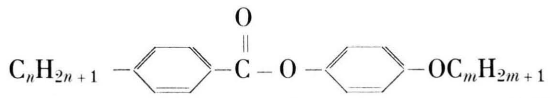
Introduction

The determination of the molecular ordering in nematic liquid crystals from their physical properties has been reported in the literature [1–19]. It is shown that the magnetic and optical methods are commonly used to study the temperature dependence of the orientational order parameters in nematic liquids.

In this work we present measurements of the diamagnetic susceptibilities, refractive indices and densities for 4-Methoxy-benzoic acid-[4′-n-pentyl-phenylester], 4-n-Hexyloxy-benzoic acid-[4′-n-pentyl-phenylester] and 4-n-Butyl-benzoic acid-[4′-n-hexyloxy-phenylester], which are of relatively low solid-nematic transition points, as a function of temperature. There are difficulties in growing single crystals from these compounds. The substances have the following structural formulas:



$m = 5;\ n = 1{,}6;$ (I, II)



$m = 6;\ n = 4.$ (III)

The Saupe-Maier model [18] is applied to the magnetic data. The Vuks formula [20, 21] and Neugebauer's relations [19, 22] are used to calculate the polarizabilities. In the former the local field is assumed to be isotropic whereas the latter implies anisotropic internal field constants.

Theoretical

The anisotropy of the diamagnetic susceptibility has been chosen by de Gennes [23] as a macroscopic property to represent the degree of ordering in nematic liquids. Such a representation for the order parameter is independent of any assumption about the rigidity of the molecules.

The anisotropic part $\boldsymbol{\chi}^{\mathrm{a}}$ of the magnetic susceptility tensor $\boldsymbol{\chi}$ could be used for defining an order parameter which is non-zero in the nematic phase but vanishes in the isotropic phase. The desired order parameter is defined [24] by

$$Q_{\alpha\beta} = \tfrac{3}{2}\, \chi^{a}_{\alpha\beta} / \Delta\chi\,, \tag{1}$$

where $\Delta\chi$ is the diamagnetic anisotropy of a perfectly ordered nematic phase. It may be derived from susceptibility measurements on a single crystal or on an ordered solid state [14]. $Q_{\alpha\beta}$ is called the macroscopic order parameter, and it is related to the microscopic order parameter S, for a nematic liquid crystal composed of rodlike molecules, by

$$Q_{\alpha\beta} = S \begin{pmatrix} -\frac{1}{2} & 0 & 0 \\ 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{2}$$

According to the Saupe-Maier model [18] we have

$$\chi_{\parallel} = \bar{\chi} + \tfrac{2}{3}\, S\, \Delta\chi\,, \tag{3 a}$$

$$\chi_{\perp} = \bar{\chi} - \tfrac{1}{3}\, S\, \Delta\chi\,, \tag{3 b}$$

where $\chi_{\parallel}$ and $\chi_{\perp}$ are the susceptibilities parallel and perpendicular to the nematic axis, respectively, and $\bar{\chi}$ is the average susceptibility. Hence,

$$S = (\chi_{\parallel} - \chi_{\perp}) / \Delta\chi\,. \tag{4}$$

The refractive index is another microscopic property by which the order parameter of nematic liquids can

Reprint requests to Prof. Dr. W. Haase, Institut für Physikalische Chemie, Technische Hochschule Darmstadt, Petersenstraße 20, *D-6100 Darmstadt.*

be represented. The relations between the principal nematic refractive indices $n_{e,o}$ and the principal polarizabilities $\alpha_{e,o}$ are given either by Vuks formula or by Neugebauer's relations. The Vuks formula for the nematic phase can be written in the form

$$\frac{n^2_{e,o}-1}{\overline{n^2}+2}\cdot\frac{M}{\varrho}=\frac{4}{3}\pi N_A\,\alpha_{e,o}=R_{e,o} \qquad (5)$$

where $\overline{n^2}=\frac{1}{3}(n_e^2+2\,n_o^2)$, M is the molecular weight, ϱ the density of the nematic phase, N_A Avogadro's number and $R_{e,o}$ are the principal molar refractions. Neugebauer's relations for the nematic phase are

$$n^2_{e,o}-1=4\pi N\,\alpha_{e,o}\,(1-N\,\alpha_{e,o}\,\gamma_{e,o})^{-1} \qquad (6)$$

and

$$\gamma_e+2\,\gamma_o=4\pi\,, \qquad (7)$$

where N is the number of molecules per cm³ in the nematic phase and $\gamma_{e,o}$ are the internal field constants.

Hence Eqs. (6) and (7) give

$$\frac{1}{\alpha_e}+\frac{2}{\alpha_o}=\frac{4\pi N}{3}\left[\frac{n_e^2+2}{n_e^2-1}+\frac{2\,(n_o^2+2)}{n_o^2-1}\right]. \qquad (8)$$

In the isotropic phase $n_e=n_o=n_i$ and we have

$$\alpha_{\|}+2\,\alpha_{\perp}=\alpha_e+2\,\alpha_o=3\,\bar{\alpha}=\frac{9}{4\pi N_i}\left[\frac{n_i^2-1}{n_i^2+2}\right] \qquad (9)$$

where $\alpha_{\|}$ and $\alpha_{\perp}$ are the principal molecular polarizabilities $\bar{\alpha}$ is the average polarizability and N_i the number of molecules per cm³ in the isotropic phase.

α_e and α_o are related to the order parameter S by relations similar to those of Eqs. (3 a) and (3 b)

$$\alpha_e=\bar{\alpha}+\tfrac{2}{3}\,S\,\Delta\alpha\,, \qquad (10\,a)$$

$$\alpha_o=\bar{\alpha}-\tfrac{1}{3}\,S\,\Delta\alpha\,, \qquad (10\,b)$$

where $\Delta\alpha$ is the anisotropy in the polarizability of an isolated molecule. Thus,

$$S=(\alpha_e-\alpha_o)/\Delta\alpha\,. \qquad (11)$$

Experimental

The diamagnetic susceptibilities were determined as functions of temperature by Faraday method at about 10 kOe. The equipment consisted of a Bruker electromagnet B-E-20 va, a Cahn RG-2000 electrobalance enclosed in a glass envelope, a Leybold-Heraeus S-16 pump and a heating system. The liquid crystal samples were sealed in quartz ampoules of uniform shape and wall thickness. The variation in the weight of the ampoules during the sealing process was about 0.5%. The sealed samples were suspended from the electrobalance by quartz fibers. The envelope was evacuated and a period of 15 – 25 minutes was allowed for the samples to reach thermal equilibrium at the desired temperature. The temperature was measured with a Chromel-Alumel thermocouple with an accuracy better than 0.2 °C. The absolute accuracy of the susceptibility measurements was about 2%, determined by the irreproducibility in the adjustment of the samples to the place where the calibration was taken and by the correction for the quartz ampoules in which the liquid crystal samples were stored.

The refractive indices were measured as functions of temperature using a Leitz microfractometer for sodium light with an error of about ±0.002. The prism was mounted in a Mettler heating stage whose temperature could be controlled electrically to an accuracy of 0.1 °C.

The density measurements were carried out as functions of temperature in a two-capillary pyc-

Table 1. Diamagnetic susceptibilities in the solid state, nematic phase and isotropic phase.

Compound I		Compound II		Compound III	
T [°C]	$(-\chi)\cdot 10^7$ [cm³ g⁻¹]	T [°C]	$(-\chi)\cdot 10^7$ [cm³ g⁻¹]	T [°C]	$(-\chi)\cdot 10^7$ [cm³ g⁻¹]
15.0	6.15	32.0	6.54	15.0	6.48
27.4	6.15	49.2	6.54	28.9	6.48
28.0	5.92	49.7	6.24	30.3	5.98
29.0 *	5.36	50.0 *	5.88	31.0 *	5.74
30.4	5.37	51.1	5.89	32.5	5.76
32.9	5.41	53.3	5.92	35.8	5.80
36.0	5.47	55.2	5.95	38.0	5.83
38.0	5.51	57.1	5.99	40.3	5.86
39.1	5.53	59.9	6.05	42.5	5.90
41.3	5.59	62.1	6.10	44.8	5.94
42.1	5.95	63.0 **	6.56	45.9	5.99
42.7 **	6.12	73.0	6.56	46.4	6.01
56.0	6.12	62.9	6.54	47.5	6.33
44.0	6.12	60.8	6.07	48.0	6.40
39.4	5.53	56.3	5.97	48.5 **	6.48
37.2	5.49	53.0	5.92	62.0	6.48
34.6	5.44	51.9	5.90	49.3	6.48
31.6	5.39			47.5	6.22
				39.6	5.85
				37.0	5.81
				33.3	5.77
				31.3	5.74

* Solid-nematic transition temperature.
** Nematic-isotropic transition temperature (T_c).

nometer of nearly 0.5 cm^3 in volume with an approximate error of ± 0.001 g/cm^3. The pycnometer was held in a thermostat whose temperature could be controlled to 0.1 °C.

Results and Discussion

Magnetic Measurements

The diamagnetic susceptibilities in the solid state, nematic phase ($\chi_{\parallel}$) and isotropic phase ($\bar{\chi}$) are reported in Table 1 as functions of temperature. These values and the values of $S\,\Delta\chi$, calculated according to Eq. (3 a), which reflect the temperature dependence of the order parameters are shown in Figures 1.

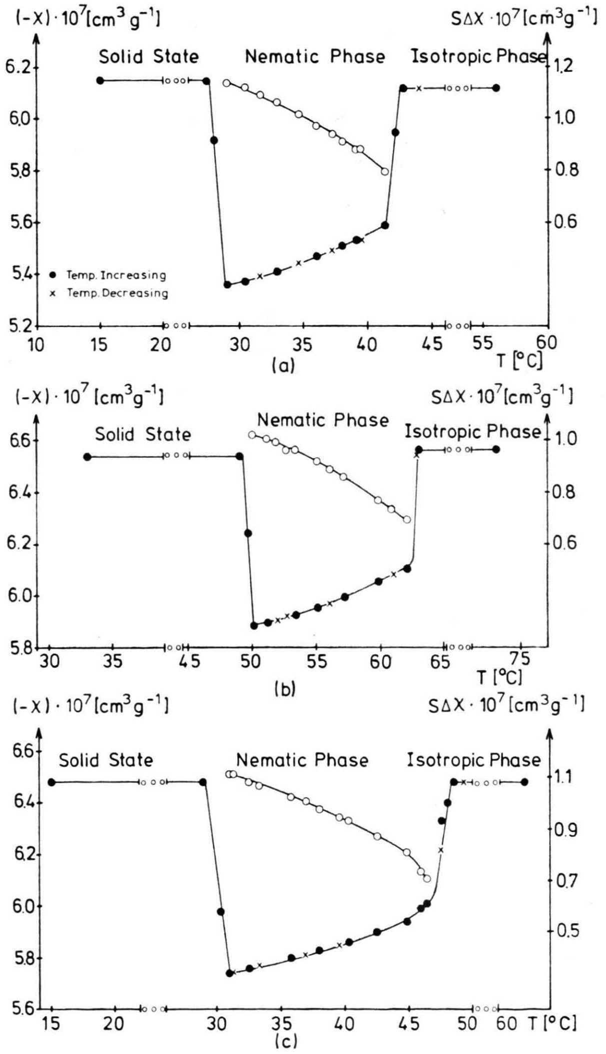


Fig. 1. Diamagnetic susceptibilities, scale on left, (● — ×) and $S\,\Delta\chi$, scale on right, (○) vs. temperature: I (a), II (b) and III (c).

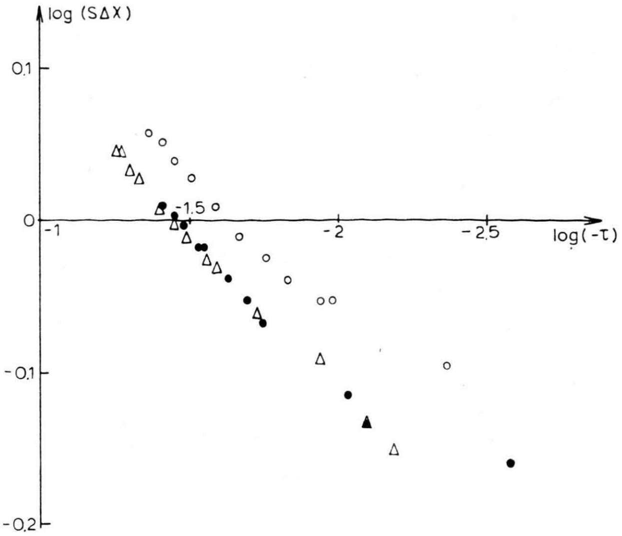


Fig. 2. Log($S\,\Delta\chi$) vs. log($-\tau$): I (○), II (●) and III (△).

We have adopted the extrapolation procedure of Haller et al.[8] plotting log ($S\,\Delta\chi$) vs. log ($-\tau$) which also gives a straight line in the temperature region $\tau < -0.016$. τ is the reduced temperature, $\tau = (T - T_c)/(T_c + 273.16)$. This plot is shown in Fig. 2 for the three compounds. The intercepts of the extrapolated straight line sections of the curves in Fig. 2 to the absolute zero ($\tau = -1$), where $S = 1$, should yield the diamagnetic anisotropies ($\Delta\chi$). The slopes of the straight lines and the molar diamagnetic anisotropies ($\Delta\chi_M$), obtained from the least-squares fits for all points in the region $\tau < -0.016$, are shown in Table 2.

Table 2. The slopes and molar diamagnetic anisotropies, obtained by extrapolating to absolute zero.

Compound	slope	$\Delta\chi_M \cdot 10^6$ [cm^3 mol^{-1}]
I	0.215	66.99
II	0.223	77.94
III	0.228	76.11

Referring to the derivation of Eq. (4), one sees that $\Delta\chi$ refers to the diamagnetic anisotropy of the molecules in the nematic phase rather than in the solid state. Therefore the values of $\Delta\chi$ obtained from the extrapolation procedure may be preferable to those from the single crystal measurements.

The increments in the mean molar susceptibility per methylene group (11.83, 12.04 and 11.78×10^{-6} cm³/mol) obtained by comparing compounds I and II, compounds II and III and compounds III and I, respectively, are in fair agreement with corresponding tabular values [25].

Density Measurements

The densities of the substances investigated are presented in Table 3 as functions of temperature The molar volumes $(\overline{V})$ of the three compounds are shown in Fig. 3 as a function of temperature. These curves show deviations from linearity in the nematic phase at about 7° below T_c. The volume expansion coefficients $[\beta \equiv (\partial \ln \overline{V}/\partial T)_p]$, calculated in the nematic phase from the least-squares fits for data with $T < (T_c - 7°)$ of $\ln \overline{V}$ vs. T, are 0.75, 0.81 and $0.77 \times 10^{-3}\,°\mathrm{C}^{-1}$ for compounds I, II, and III, respectively. The least-squares fits for all points in the isotropic phase result in β's of 0.80, 0.83 and $0.81 \times 10^{-3}\,°\mathrm{C}^{-1}$ for I, II and III, respectively.

Assuming that the molar volume is a simple additive function of the atomic volumes, the increments in the molar volume per methylene group (17.16 and 17.50 cm³/mol) are deduced by comparing compounds I and II in the nematic phase at 6° below T_c and in the isotropic phase at 5° above T_c, respectively. The contribution of the methylene group has been evaluated in 4,4′-disubstituted α-chlorostilbene [8] (16.34 cm³/mol) in the nematic phase, in n-alkanes [26], alkylbenzenes [27] and alkylbiphenyls [28] (16.4, 16.6 and 17.1 cm³/mol, respectively) in the isotropic phase and in n-alkanes [26] (14.5 cm³/mol) in the solid state.

Optical Measurements

The indices of refraction for sodium light in the nematic and isotropic phases are also reported in Table 3. These values and $S\,\Delta\alpha$, which reflect the variation of the molecular ordering in the nematic phase, deduced according to Eq. (11) applying either Neugebauer's relations or Vuks formula are shown in Figures 4.

The internal field constants (γ_e) exhibit a minimum at nearly the middle of the nematic ranges. γ_e values for compounds I and II, which are from the same homologous series, appear to be identical at the same $(T_c - T)$. In the case of compound III,

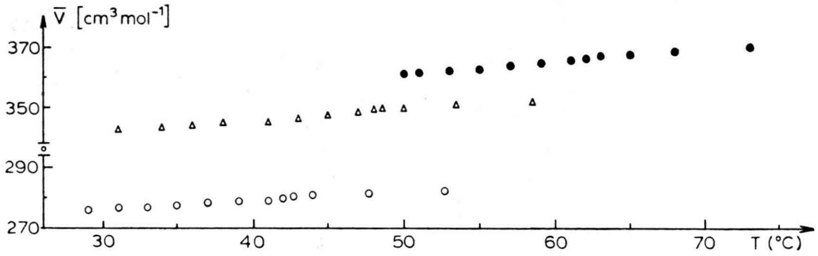


Fig. 3. Molar volumes vs. temperature: I (○), II (●), and III (△).

Table 3. Densities and refractive indices, for sodium light, in the liquid crystalline and isotropic phases.

Compound I				Compound II				Compound III			
T[°C]	ϱ[g/cm³]	n_o	n_e	T[°C]	ϱ[g/cm³]	n_o	n_e	T[°C]	ϱ[g/cm³]	n_o	n_e
29.0	1.080	1.513	1.649	50.0	1.019	1.490	1.613	31.0	1.033	1.496	1.615
31.0	1.078	1.514	1.645	51.0	1.018	1.490	1.611	34.0	1.030	1.496	1.612
33.0	1.077	1.514	1.643	53.0	1.016	1.490	1.607	36.0	1.029	1.497	1.608
35.0	1.075	1.515	1.639	55.0	1.015	1.491	1.602	38.0	1.027	1.497	1.604
37.0	1.072	1.515	1.633	57.0	1.012	1.492	1.598	41.0	1.025	1.498	1.599
39.0	1.070	1.517	1.629	59.0	1.009	1.493	1.592	43.0	1.022	1.498	1.596
41.0	1.068	1.519	1.620	61.0	1.007	1.496	1.583	45.0	1.018	1.498	1.592
42.0	1.066	1.522	1.613	62.0	1.005	1.498	1.577	47.0	1.016	1.501	1.583
42.7	1.063	1.550	1.550	63.0	1.002	1.522	1.522	48.0	1.014	1.503	1.577
44.0	1.061	1.550	1.550	65.0	1.001	1.521	1.521	48.5	1.013	1.527	1.527
47.7	1.059	1.548	1.548	68.0	0.998	1.520	1.520	50.0	1.012	1.526	1.526
52.7	1.054	1.546	1.546	73.0	0.994	1.518	1.518	53.5	1.008	1.524	1.524
								58.5	1.005	1.522	1.522

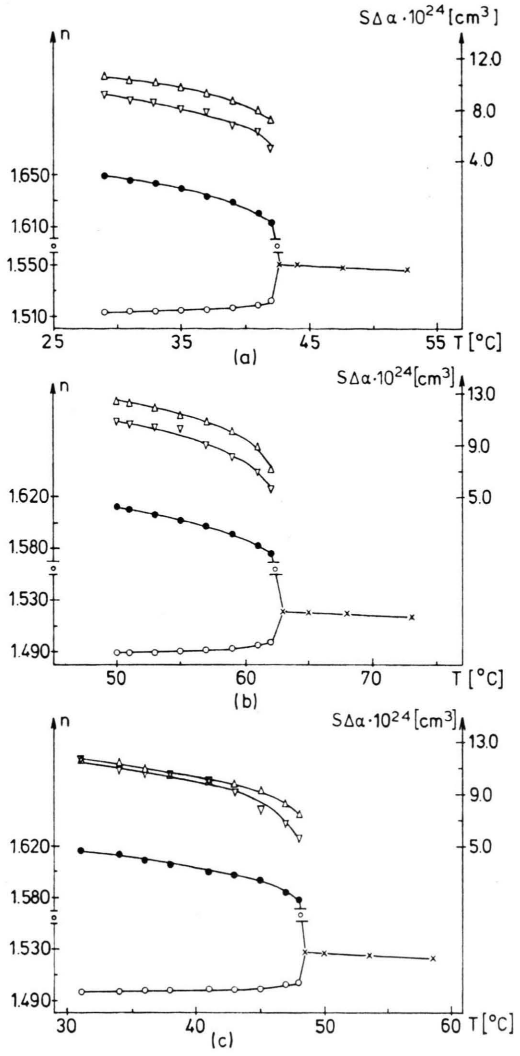


Fig. 4. Refractive indices n_o (○), n_e (●) and n_i (×), scale on left, and $S\,\Delta\alpha$ obtained from Vuks formula (△) and from Neugebauer's relations (▽), scale on right, vs. temperature: I (a), II (b) and III (c).

γ_e's have a mean value (3.62) in the temperature range $(T_c - T) > 5^\circ$ compared with 3.79 for I and II in the same range. For the three compounds, the values of γ_e are approximately equal in the temperature range $(T_c - T) < 5^\circ$ and have a mean value of 4.03.

The extrapolation procedure of Haller et al. [8] is adopted here using the polarizabilities calculated from Vuks formula. The plot of log $(S\,\Delta\alpha)$ vs. log $(-\tau)$ for the three compounds is shown in Figure 5. The molecular polarizability anisotropies $(\Delta\alpha_V)$ obtained from the least-squares fits for the data in the temperature range $\tau < -0.016$, are listed in Table 4. A similar extrapolation for anisaldazine, using the refractive index and density data of Madhusudana et al. [9], yields $\Delta\alpha_V = 37.3 \times 10^{-24}$ cm³. This value is 6 per cent lower than the value 39.7 $\times 10^{-24}$ cm³ obtained from the single crystal data [9].

Table 4. The molecular polarizabilities and polarizability anisotropies, for sodium light, obtained by extrapolating to absolute zero.

Compound	$\Delta\alpha_V \cdot 10^{24}$ [cm³]	$\alpha_{\parallel} \cdot 10^{24}$ [cm³]	$\alpha_{\perp} \cdot 10^{24}$ [cm³]	$\Delta\alpha_N \cdot 10^{24}$ [cm³]
I	16.90	44.90	30.75	14.15
II	23.23	56.20	38.63	17.57
III	18.78	53.76	37.12	16.64

Using the polarizabilities from Neugebauer's relations, we have adopted the extrapolation procedure of Subramhanyam et al. [19]. Figure 6 shows the curves of $\log(\alpha_e/\alpha_o)$ versus $\log(T_c - T)$ for the investigated substances. The molecular polarizabilities $\alpha_{\parallel}$ and $\alpha_{\perp}$ and the anisotropy in the polarizability $(\Delta\alpha_N)$, obtained from the least-squares fits for data points with $(T_c - \Theta > 5^\circ$, are also reported in Table 4. A similar extrapolation for anisaldazine, using the same data as before, yields $\alpha_{\parallel} = 55.40 \times 10^{-24}$ cm³, $\alpha_{\perp} = 27.05 \times 10^{-24}$ cm³ and $\Delta\alpha_N = 28.35 \times 10^{-24}$ cm³ in a good agreement with the single crystal data [19] (55.82, 26.84 and 28.98 $\times$ 10^{-24} cm³, respectively).

By comparing compounds I and II in the nematic phase, at about 6° below T_c, an increment of 4.6 cm³/mol in the mean molar refraction per methylene group is evaluated. This value is in a good agreement with 4.7 cm³/mol found by Kovshik et al. [29]. The increments per methylene group in the mean molecular polarizabilities (1.81, 1.84 and 1.80 $\times$ 10^{-24} cm³) are obtained by comparing I and II, II and III and III and I, respectively, in the isotropic phase, at 5° above T_c. The agreement with 1.88×10^{-24} cm³ reported by Haller et al. [8] is satisfactory.

Order Parameters

The orientational order parameters calculated from the magnetic data (S) and from the optical data $(S_V$ and $S_N)$ using the two approaches are summarized as functions of temperature in Table 5. The Vuks formula and Neugebauer's relations lead

Table 5. Order parameters calculated from the magnetic and from the optical data.

							Magnetic							
I	T[°C]	29.0	30.4	31.6	32.9	34.6	36.0	37.2	38.0	39.1	39.4	41.3		
	S	0.51	0.50	0.49	0.47	0.45	0.43	0.42	0.41	0.39	0.39	0.36		
II	T[°C]	50.0	51.1	51.9	53.0	53.3	55.2	56.3	57.1	59.9	60.8	62.1		
	S	0.48	0.48	0.47	0.45	0.45	0.43	0.42	0.40	0.36	0.35	0.33		
III	T[°C]	31.0	31.3	32.5	33.3	35.8	37.0	38.0	39.6	40.3	42.5	44.8	45.9	46.4
	S	0.52	0.52	0.50	0.50	0.48	0.47	0.45	0.44	0.43	0.41	0.38	0.34	0.33
							Optical							
I	T[°C]	29.0	31.0	33.0	35.0	37.0	39.0	41.0	42.0					
	S_V	0.63	0.61	0.60	0.58	0.55	0.52	0.47	0.42					
	S_N	0.65	0.61	0.61	0.57	0.55	0.47	0.45	0.35					
II	T[°C]	50.0	51.0	53.0	55.0	57.0	59.0	61.0	62.0					
	S_V	0.54	0.53	0.52	0.49	0.47	0.44	0.39	0.35					
	S_N	0.61	0.61	0.60	0.59	0.52	0.46	0.40	0.32					
III	T[°C]	31.0	34.0	36.0	38.0	41.0	43.0	45.0	47.0	48.0				
	S_V	0.62	0.60	0.58	0.56	0.53	0.51	0.49	0.43	0.39				
	S_N	0.69	0.64	0.63	0.62	0.59	0.54	0.46	0.40	0.33				

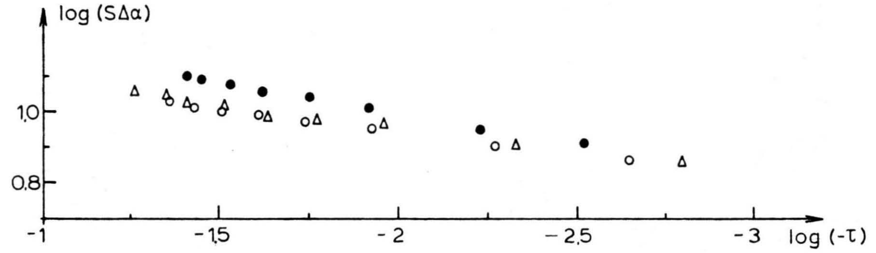


Fig. 5. Log($S\,\Delta\alpha$) vs. log($-\tau$) : I (○), II (●) and III (△).

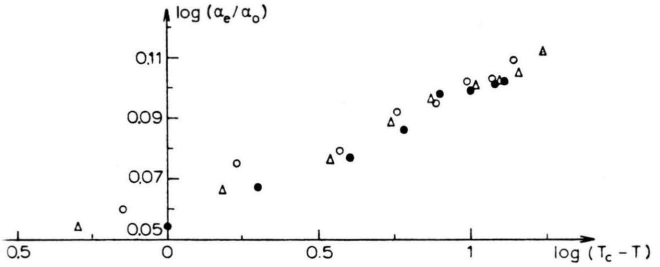


Fig. 6. Log(α_e/α_o) vs. log($T_c - T$) : I (○), II (●) and III (△).

to comparable values for the order parameters, however, the former does not concern with the anisotropy of the local field. The values of S_N are in all cases lower than S_V in the vicinity of the nematic-isotropic transition temperature.

The definition of the order parameter through the diamagnetic anisotropy is preferable. This is because the induced magnetic dipoles do not interact appreciably whereas the optically induced dipoles are so strong as to exert a considerable interaction on one another. Taking this limitation and the probable errors into account, the order parameters obtained from the magnetic and from the optical data can be compared. The values from the optical data are markedly higher than those from the magnetic data. The order parameters obtained from Neugebauer's relations are slightly in better agreement with those from the magnetic data in the vicinity of T_c. The differences between S_V and the corresponding S values are nearly equal for each compound in the whole nematic range.

It may be shown that the curves for the order parameters versus temperature, obtained either from the magnetic data or from the optical data, are nearly parallel for those compounds in the same homologous series.

Acknowledgements

The authors appreciate the financial support of the Deutsche Forschungsgemeinschaft. – We thank Dr. J. Krause, E. Merck, Darmstadt, for providing compounds.

[1] V. Zwetkoff, Acta Physicochimica (URSS) **16,** 132 [1942].

[2] P. Chatelain, Bull. Soc. France Miner. Crist. **78,** 262 [1955].

[3] R. Alben, J. R. McColl, and C. S. Shih, Solid State Commun. **11,** 1081 [1972].

[4] S. Chandrasekhar and N. V. Madhusudana, Mol. Cryst. Liq. Cryst. **10,** 151 [1970].

[5] R. Chang, Mol. Cryst. Liq. Cryst. **30,** 155 [1975].

[6] P. Delord, J. Phys. Paris **30,** C4-14 [1969].

[7] H. Gasparoux, B. Regaya, and J. Prost, C. R. Acad. Sci. (Paris) **B 272,** 1168 [1971].

[8] I. Haller, H. A. Huggins, H. R. Lilienthal, and T. R. McGuire, J. Phys. Chem. **77,** 950 [1973].

[9] N. V. Madhusudana, R. Shashidhar, and S. Chandrasekhar, Mol. Cryst. Liq. Cryst. **13,** 61 [1971].

[10] J. R. McColl, Phys. Lett. A **38,** 55 [1972].

[11] J. R. McColl and C. S. Shih, Phys. Rev. Lett. **29,** 85 [1972].

[12] V. D. Neff, L. W. Gulrich, and G. H. Brown, Mol. Cryst. Liq. Cryst. **1,** 225 [1966].

[13] Y. Poggi, G. Labrunie, and J. Robert, C. R. Acad. Sci. (Paris) **B 277,** 561 [1973].

[14] Y. Poggi, J. Robert, and J. Borel, Mol. Cryst. Liq. Cryst. **29,** 311 [1975].

[15] V. G. Rumyantsev, P. D. Berezin, L. M. Blinov, and I. Kompanets, Kristallografiya **18,** 1104 [1973].

[16] V. G. Rumyantsev, L. M. Blinov, and V. A. Kizel, Kristallografiya **18,** 1101 [1973].

[17] A. Saupe, Angew. Chem. **80,** 99 [1968].

[18] A. Saupe and W. Maier, Z. Naturforsch. **16 a,** 816 [1961].

[19] H. S. Subramhanyam, C. S. Prabha, and D. Krishnamurti, Mol. Cryst. Liq. Cryst. **28,** 201 [1974].

[20] M. F. Vuks, Optics and Spectroscopy **20,** 361 [1966].

[21] S. Chandrasekhar and N. V. Madhusudana, J. Phys. (Paris), Suppl. **30,** C4-24 [1969].

[22] H. E. J. Neugebauer, Can. J. Phys. **32,** 1 [1954].

[23] P. G. de Gennes, Mol. Cryst. Liq. Cryst. **12,** 193 [1971].

[24] E. B. Priestley, P. J. Wojtowicz, and P. Sheng, "Introduction to Liquid Crystals", Plenum Press, New York 1974, 1975, p. 75.

[25] A. Weiss and H. Witte, "Magnetochemie", Verlag Chemie, Weinheim (Bergstraße) 1973, p. 77.

[26] S. S. Kurtz, in "The Chemistry of Petroleum Hydrocarbons", Vol. 1, B. T. Brooks et al., Ed., Reinhold, New York 1954, p. 275.

[27] J. Timmermans, "Physico-chemical Constants of Pure Organic Compounds", Elsevier Publishing Co., Amsterdam 1965.

[28] I. A. Goodman and P. K. Wise, J. Amer. Chem. Soc. **72,** 3076 [1950].

[29] A. P. Kovshik, Yu. I. Denite, and E. I. Ryumtsev, Kristallografiya **20,** 861 [1975].