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Properties of the discotic-nematic to isotropic transition: influence of short range orientational order

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The present investigation concerns the analysis of the influence of short range orientational correlation on the thermodynamic properties of discotic-nematic liquid crystals. Two-site cluster approximation is applied to the orientational molecular coordinates to include the short range orientational correlation. The role of short range orientational order, dispersion interaction, molecular length-to-width ratio and pressure on the thermodynamic and orientational behaviour of discotic nematogens close to the discotic-nematic to isotropic transition are analysed. It is observed that the short range orientational order has a strong influence on the thermodynamic properties and that the transition properties of both the calamitic and discotic mesogens exhibit quite similar behaviour.

1. Introduction

In a previous paper [1] we investigated the influence of short range orientational correlation on the thermodynamic and orientational properties of calamitic-nematic liquid crystals. The work was based on the application of a perturbation theory [2] and a two-site cluster (TSC) approximation [3, 4] to treat the orientational molecular coordinates so as to include the short range orientational order. It was found that the short range orientational order has a strong influence on the calamitic-nematic to isotropic transition properties and that the numerical results are in better agreement with experiments than in our earlier work [2*a*] where a mean-field (MF) approximation was used. In the present work we study the effect of short range orientational order on the thermodynamic and orientational behaviour of discotic nematogens [5] close to the discotic-nematic to isotropic (N_D -I) phase transition by extending the theory as used in ref. [1].

In order to account for nearest-neighbour correlation between molecular orientations, at least a two-particle orientational distribution function is required. A cluster-variation method known from the theory of ferromagnetism provides such a distribution in a simple way. A TSC approximation based on a lattice version of the Maier-Saupe model includes some nearest-neighbour correlation between molecular orientations. In the following section, a brief outline of theory and working equations is given. The results and discussion are given in § 3.

2. Theory and working equations

We consider a system composed of N discotic-nematic molecules of axial symmetry contained in volume V at temperature T interacting through a potential function given by

$$U_N(X_1, X_2) = \sum_{1 \leq i < j \leq N} [U_0(X_i, X_j) + U_p(X_i, X_j)]$$

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where the vector $X_i[\equiv (r_i, \Omega_i)]$ represents both the location r_i of the centre of mass of the i th molecule and its relative orientation Ω_i described by Euler's angles θ_i , ϕ_i and ψ_i . The reference potential U_0 is described by the repulsion between the hard ellipsoids of revolution, and satisfies the relation

$$U_0(X_1, X_2) = U_{\text{her}}(X_1, X_2) = \begin{cases} \infty, & \text{for } r_{12} \leq D(\widehat{r}_{12}, \Omega_{12}) \\ 0 & \text{for } r_{12} > D(\widehat{r}_{12}, \Omega_{12}). \end{cases} \quad (2)$$

U_p represents the perturbation potential which contains a smoothly varying long range attractive part and is described by the dispersion interaction:

$$U_p(X_1, X_2) = U_0(r_{12}, \Omega_1, \Omega_2) = \begin{cases} r_{12}^{-6} [C_i + C_a P_2(\widehat{e}_1 \cdot \widehat{e}_2)] & \text{for } r_{12} > D(\widehat{r}_{12}, \Omega_{12}) \\ 0 & \text{for } r_{12} \leq D(\widehat{r}_{12}, \Omega_{12}). \end{cases} \quad (3)$$

Here $D(\widehat{r}_{12}, \Omega_{12})$ is the distance of closest approach between two molecules with relative orientation Ω_{12} . \widehat{r}_{12} is a unit vector along the intermolecular axis and $\widehat{e}_1, \widehat{e}_2$ are the unit vectors along the symmetry axes of two interacting molecules. C_i and C_a are constants related to the isotropic and anisotropic dispersion interactions, respectively. We consider the following form [6] for $D(\widehat{r}_{12}, \Omega_{12})$:

$$D(\widehat{r}_{12}, \Omega_{12}) = d_0 \left[1 - \chi \frac{(\widehat{r}_{12} \cdot \widehat{e}_1)^2 + (\widehat{r}_{12} \cdot \widehat{e}_2)^2 - 2\chi(\widehat{r}_{12} \cdot \widehat{e}_1)(\widehat{r}_{12} \cdot \widehat{e}_2)(\widehat{e}_1 \cdot \widehat{e}_2)}{1 - \chi^2(\widehat{e}_1 \cdot \widehat{e}_2)^2} \right]^{-1/2} \quad (4)$$

where $d_0 (= 2b)$ is the molecular diameter and $\chi = X_0^2 - 1/X_0^2 + 1$ where X_0 is the length-to-width ratio.

Assuming the pairwise additivity of the interaction potential and adopting the procedure as outlined in [2a], the perturbation series for the Helmholtz free energy is written as

$$\frac{\beta A}{N} = \frac{\beta(A)^0}{N} + \sum_{s=0}^{\infty} \frac{\beta A^{(s)}}{N} \quad (5)$$

where A^0 is the contribution of the reference system and

$$\frac{\beta A^{(s)}}{N} = \beta \int f(\Omega_1) d\Omega_1 \psi^0 \Omega_1 \quad (6)$$

represents the perturbation terms. $f(\Omega_1)$ is the one-particle orientational distribution function, s denotes the order of perturbation and $\psi^{(s)}$ is defined as an effective one-body orientational perturbation potential given by

$$\psi^{(s)}(\Omega_1) = \frac{1}{2^s \rho} \int f(\Omega_2) d\Omega_2 \times \int d\widehat{r}_{12} u_p(\widehat{r}_{12}, \Omega_1, \Omega_2) g^{(s-1)}(\widehat{r}_{12}, \Omega_1, \Omega_2). \quad (7)$$

Here $g^{(s-1)}(\widehat{r}_{12}, \Omega_1, \Omega_2)$ is the pair correlation function for all s . For $s = 1$, $g^{(0)}(\widehat{r}_{12}, \Omega_1, \Omega_2)$ represents the PCF for reference system.

In order to calculate the thermodynamic properties of a system of hard ellipsoids, we start with the pressure relation

$$\frac{\beta p_0}{\rho} = 1 - \frac{\beta \rho}{6} \int d\widehat{r}_{12} \int f(\Omega_1) d\Omega_1 \int f(\Omega_2) d\Omega_2 \times [\widehat{r}_{12} \nabla u_{\text{her}}(\widehat{r}_{12}, \Omega_1, \Omega_2) g^0(\widehat{r}_{12}, \Omega_{12})]. \quad (8)$$

The operator ∇ acts on the r_{12} coordinates of $u_{\text{her}}(\widehat{r}_{12}, \Omega_1, \Omega_2)$ only. The above equation is evaluated using a decoupling approximation [7] which amounts to the assumption

$$g^{(0)}(\widehat{r}_{12}, \Omega_{12}) = g^{(0)} \frac{\widehat{r}_{12}}{D(\widehat{r}_{12}, \Omega_{12})} = g^{(0)}(r_{12}^*). \quad (9)$$

This approximation completely decouples the orientational and positional degree of freedom. Also, in solving equation (8) we consider excluded volume, or co-volume, between the two ellipsoids of revolution

$$V_{\text{exc}}(\Omega_{12}) = \frac{1}{3} \int D^3(\widehat{r}_{12}, \Omega_{12}) d\widehat{r}_{12} = 8v_0(1 - \chi^2)^{-1/2}(1 - \chi^2 \cos^2 \theta_{12})^{1/2}. \quad (10)$$

v_0 is the volume of a molecule and θ_{12} is the angle between the axes of molecules. Considering the Berne and Pechukas relation [6] for $D(\widehat{r}_{12}, \Omega_{12})$ as given in equation (4), reducing the distance variable with $D(\widehat{r}_{12})$ and using equation (9), we get

$$\frac{\beta p_0}{\rho} = 1 + \frac{2\eta(2 - \eta)}{(1 - \eta)^3} [F_0(\chi) - F_2(\chi)P_2^2] \quad (11)$$

where, $\eta = \rho v_0$, η is the packing fraction [8] and ρ is the number density.

$$F_0(\chi) = (1 - \chi^2)^{-1/2} \left[1 - \frac{1}{6}\chi^2 - \frac{1}{40}\chi^4 - \frac{1}{112}\chi^6 \dots \right] \quad (12)$$

$$F_2(\chi) = \frac{1}{3}\chi^2(1 - \chi^2)^{-1/2} \left[1 + \frac{3}{14}\chi^2 + \frac{5}{56}\chi^4 + \frac{25}{528}\chi^6 + \dots \right] \quad (13)$$

$$\bar{P}_n = \int f(\Omega) d\Omega P_n(\cos \theta). \quad (14)$$

The Helmholtz free energy per particle for the reference system can be written by using standard thermodynamic relations and we get finally

$$\frac{\beta A^0}{N} = (\ln \rho - 1) + \langle \ln [4\pi f(\Omega)] \rangle + \frac{\eta(4 - 3\eta)}{(1 - \eta)^2} [F_0(\chi) - F_2(\chi)\bar{P}_2^2]. \quad (15)$$

The Helmholtz free energy in the first order perturbation is

$$\frac{\beta A^{(1)}}{N} = \beta \int f(\Omega) d\Omega \psi^{(1)}(\Omega). \quad (16)$$

All symbols have their usual meaning as stated earlier. Reducing the distance variables with $D(\Omega_{12})$, considering the expression for $D(\bar{r}_{12}, \Omega_{12})$ and solving the integrals involved, we write

$$\frac{\beta A^{(1)}}{N} = \beta(-\phi_0 - \phi_2\bar{P}_2^2) \quad (17)$$

where

$$\phi_0 = \left(\frac{\pi x_0}{12} \right) \eta I_6(\eta) C_{id}^* \left[A_0 + \frac{1}{5} \left(\frac{C_{ad}^*}{C_{id}^*} \right) A_2 \right] \quad (18)$$

$$\phi_2 = \left(\frac{\pi x_0}{12} \right) \eta I_6(\eta) C_{id}^* \left[A_4 + \left(A_0 + \frac{2}{7} A_2 \right) \frac{C_{ad}^*}{C_{id}^*} \right] \quad (19)$$

with $c_{id}^* = c_{id}/v_0^2$ and $c_{ad}^* = c_{ad}/v_0^2$. A_0 , A_2 and A_4 are the constants appearing in the integral $I_6(\eta)$ defined by

$$I_6(\rho, T) = \int_0^\infty r_{12}^{*-4} g_{hs}^{(0)}(r_{12}^*) dr_{12}^*.$$

Here $g_{hs}^{(0)}$ is the pair correlation function for a hard sphere and the above integral is evaluated from the series proposed by Larsen *et al.* [9]. With the help of equations (15) and (16) the total configurational

Helmholtz free energy can be written as

$$\frac{\beta A}{N} = B_0(\eta, T) + \frac{\beta A_{orient}}{N} \quad (20)$$

where B_0 is the orientation independent contribution.

$$B_0(\eta, T) = \ln \rho - 1 + \frac{\eta(4 - 3\eta)}{(1 - \eta)^2} F_0(\chi) - \beta \phi_0 \quad (21)$$

and A_{orient} refers to the orientational free energy.

$$\frac{\beta A_{orient}}{N} = \langle \ln [4\pi f(\Omega)] \rangle - B_2(\eta, T)\bar{P}_2^2 \quad (22)$$

where $B_2(\eta, T) = (\eta(4 - 3\eta)/(1 - \eta)^2)F_2(\chi) + \beta\phi_2$. In the MF approximation used in ref. [2b] the molecular orientation is expressed in terms of the one-particle orientation distribution function and the short range orientational correlation is neglected. The TSC approximation provides a two-particle orientational distribution function of the form

$$f(\Omega_1, \Omega_2) = \frac{1}{z_{12}} \exp \left\{ \frac{B_2(\eta, T)}{\gamma} P_2(\hat{e}_1 \cdot \hat{e}_2) + \frac{\gamma - 1}{\gamma} B_2(\eta, T) \bar{S} [P_2(\widehat{r}_{12} \cdot \hat{e}_1) + P_2(\widehat{r}_{12} \cdot \hat{e}_2)] \right\} \quad (23)$$

where

$$z_{12} = \int d\Omega_1 d\Omega_2 \exp \left\{ \frac{B_2(\eta, T)}{\gamma} P_2(\hat{e}_1 \cdot \hat{e}_2) + \frac{\gamma - 1}{\gamma} B_2(\eta, T) \bar{S} [P_2(\widehat{r}_{12} \cdot \hat{e}_1) + P_2(\widehat{r}_{12} \cdot \hat{e}_2)] \right\} \quad (24)$$

and γ denotes the number of nearest neighbours of a molecule. The orientational free energy of the system in the TSC approximation is obtained as

$$\frac{\beta A_{orient}}{N} = -\frac{1}{2}\gamma \ln z_{12} + (\gamma - 1) \ln z_1 \quad (25)$$

where $z_1 = \int d\Omega \exp [2B_2(\eta, T) \bar{S} P_2(\widehat{r}_{12} \cdot \hat{e}_1)]$. Obviously, the one-particle distribution function in this case is

$$f(\Omega) = \frac{1}{z_1} \exp [2B_2(\eta, T) \bar{S} P_2(\widehat{r}_{12} \cdot \hat{e}_1)]. \quad (26)$$

In the above expression \bar{S} is a variational parameter which is determined self-consistently by minimizing the free energy. The result is

$$\frac{1}{2} \langle [P_2(\widehat{r}_{12} \cdot \hat{e}_1) + P_2(\widehat{r}_{12} \cdot \hat{e}_2)] \rangle_{z_{12}} = \langle P_2(\widehat{r}_{12} \cdot \hat{e}_1) \rangle_{z_1}. \quad (27)$$

Here the thermal averages $\langle \dots \rangle_{z_{12}}$ and $\langle \dots \rangle_{z_1}$ must be evaluated, respectively with the two- and one-particle distribution functions given above. The total Helmholtz free energy per particle in the TSC approximation is given by

$$\frac{\beta A}{N} = B_0(\eta, T) - \frac{1}{2} \gamma \ln z_{12} + (\gamma - 1) \ln z_1. \quad (28)$$

Thermodynamic quantities such as pressure, chemical potential and entropy can readily be derived from equation (28). In these expressions there appears a term $\langle P_2(\widehat{e}_1, \widehat{e}_2) \rangle_{z_{12}}$ which measures the nearest-neighbours correlation in the molecular orientation. This quantity is defined as a short range orientational order parameter

$$\bar{\sigma} = \langle P_2(\widehat{e}_1, \widehat{e}_2) \rangle_{z_{12}}. \quad (29)$$

The discotic-nematic to isotropic (N_D -I) transition is located by equating the pressures and chemical potentials of the two phases.

3. Results and discussion

We have analysed the influence of the short range orientational order $\bar{\sigma}$, interaction parameters (C_i and C_a) and the length-to-width ratio x_0 on a variety of thermodynamic and orientational properties of discotic nematics close to the N_D -I phase transition. Figure 1 shows the transition temperature as a function of isotropic

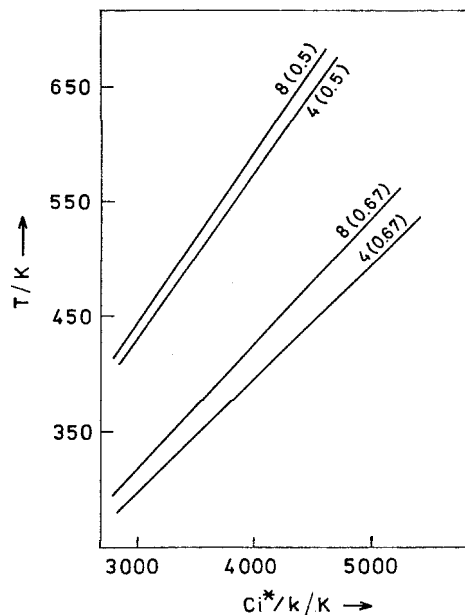


Figure 1. The variation of N_D -I transition temperature T at fixed $C_i^*/C_a^* = 10$ as a function of C_i^*/k for several numbers of nearest-neighbours γ . The number on the curve indicates the value of γ and the number in the small bracket indicates the two values of x_0 .

attraction C_i for a fixed C_a . The curves are drawn for several numbers of nearest-neighbours γ . The transition temperatures, for fixed C_i and C_a , are plotted as a function of γ in figure 2. In the table, a number of transition properties at atmospheric pressure are compared with the results obtained for several values of γ and the MF result [2*b*]. The variation of density, relative density change, long range and short range order parameters are shown in figure 3 as a function of γ . The parameter Γ listed in the table measures the relative sensitivity of the long range order parameter to volume change (at constant temperature) and temperature change (at constant volume). The pressure dependence of the transition temperature dT_{N_D-I}/dp is determined by the Clausius-Clapeyron Law.

It transpires from the table that the transition temperature changes with the change of short range order in the TSC approximation. The transition temperature increases with decrease of short range order. Its value is approximately 1/10th of the interaction parameter C_i^*/k . We observe also that the transition temperature has a smaller value in the TSC approximation compared with the MF approximation where short range order was not considered. The discontinuities in the longer range order parameter, and the density and entropy at the transition, decrease on the inclusion of a short range orientational correlation in the calculation. The transition is strongly influenced by the number of nearest neighbours γ . As γ increases the phase transition

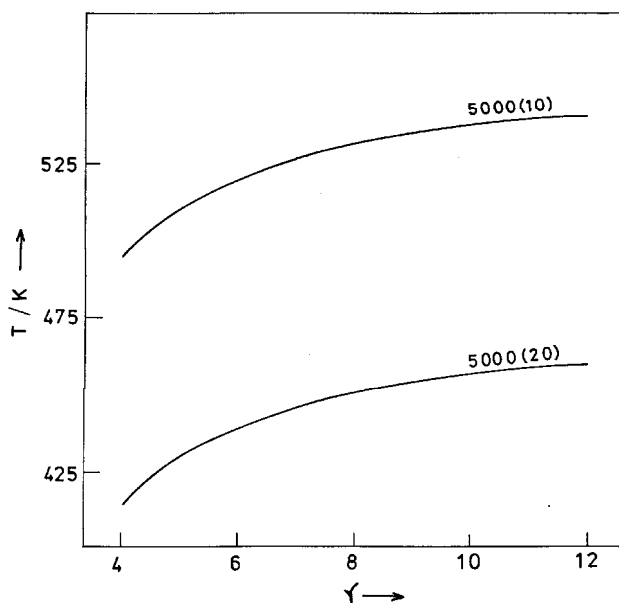


Figure 2. The variation of N_D -I transition temperature T at fixed C_i^*/k and C_i^*/C_a^* as a function of nearest-neighbours γ . The number on the curve indicates the value of C_i^*/k and the number in the small bracket indicates the value of C_i^*/C_a^* .

Table The discotic-nematic to isotropic transition parameter for $x_0 = 0.67$ as predicted by the TSC approximation for various numbers of nearest-neighbours γ . $\bar{P}_{2N_D I}$ is the long range order parameter, $\bar{\sigma}_{N_D I}$ is the short range order parameter, η the nematic packing fraction, $\Delta\eta/\eta$ is the relative density change, $\Delta\Sigma/Nk$ is the transition entropy.

$\frac{C_i^*}{k}$	$\frac{C_i}{C_a}$	γ	$T_{N_D I}$	$\bar{P}_{2N_D I}$	$\bar{\sigma}_{N_D I}$	η	$\frac{\Delta\eta}{\eta}$	$\frac{\Delta\Sigma}{Nk}$	$\left(\frac{dT_{N_D I}}{dp}\right)_{p=1 \text{ bar}}$	Γ	
5000	10	4	494.6	0.428	0.486	0.573	0.015	0.031	143.5	2.06	
		6	521.5	0.468	0.402	0.557	0.022	0.41	167.2	2.04	
		8	533.2	0.487	0.366	0.549	0.026	0.45	177.5	2.03	
		12	541.1	0.501	0.334	0.544	0.029	0.49	186.7	2.01	
	MF (Ref. [2b])	—	—	587.0	0.541	—	0.509	0.044	1.25	118.5	1.85
		20	4	413.8	0.430	0.486	0.609	0.010	0.27	102.4	2.24
			6	440.0	0.471	0.401	0.589	0.014	0.34	118.6	2.22
			8	451.5	0.491	0.365	0.588	0.017	0.38	125.4	2.20
			12	461.1	0.508	0.333	0.577	0.018	0.41	131.7	2.19

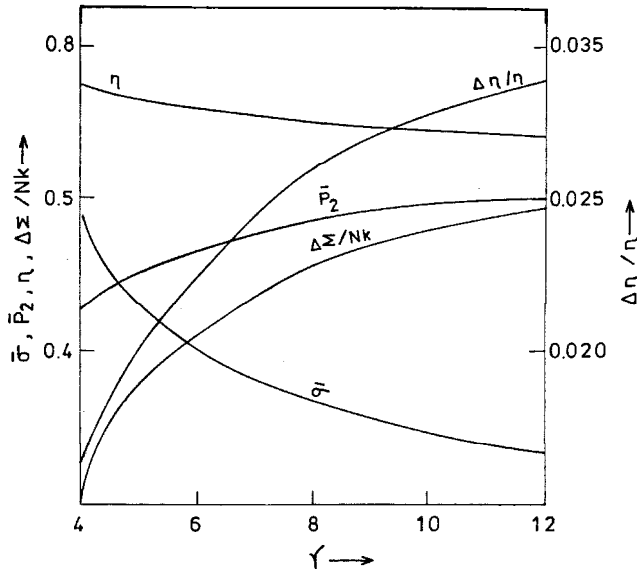


Figure 3. The variation of packing fraction η , long range orientational order parameter $\bar{P}_{2N_D I}$, short range order parameter $\bar{\sigma}_{N_D I}$ and the relative density change $\Delta\eta/\eta$ at the N_D -I transition as a function of number of nearest-neighbours γ for the parameter $x_0 = 0.67$, $C_i^*/k = 5000(k)$ and $C_i^*/C_a^* = 10$.

shifts to a higher temperature and lower density, with increasing discontinuities in long range order parameter, density and entropy. The value of the short range order parameter decreases with γ but the parameter Γ remains almost unaffected.

The variation of transition properties (not shown in the table) with the strengths of the potential parameters C_i and C_a for the several values of x_0 have been studied. We find that for a given Γ with increasing x_0 the phase transition is at a higher temperature, lower density, with higher entropy and density changes and a jump in order parameters.

The interaction parameters also have a strong influence on the transition properties. For a fixed ratio

C_i/C_a , as C_i increases the transition temperature increases, whereas the order parameters and discontinuities in the density and entropy decrease. From the table it is clear that for a given value C_i , as the ratio C_i/C_a increases the relative density change decreases. The packing fraction η increases with C_i/C_a but the increase is slow. For $C_i/C_a > 20$, we find that the transition properties are less sensitive to this ratio. Figure 4 shows the temperature dependence of order parameter \bar{P}_2 and $\bar{\sigma}$ at constant pressure ($p = 1$ bar); the TSC and MF results are compared. The difference between TSC and MF results is clearly seen in the isotropic phase where the long range order \bar{P}_2 vanishes but the short range order $\bar{\sigma}$ is still non-zero.

We have studied the pressure dependence of the thermodynamic parameters for the N_D -I transition; detailed results are not given here. Significant results are listed as follows:

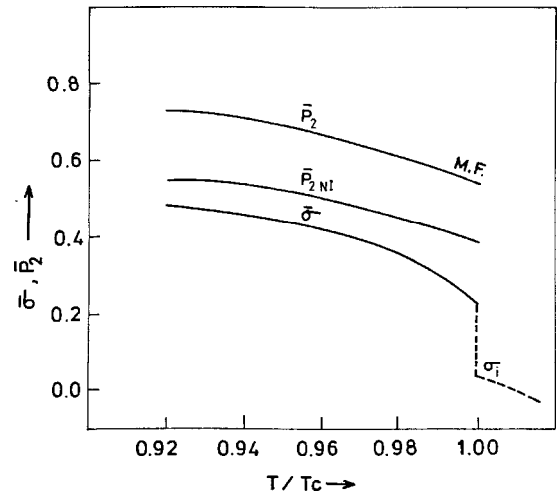


Figure 4. The temperature variation of order parameters \bar{P}_2 and $\bar{\sigma}$ at constant pressure compared with mean-field results.

- (1) The range of the discotic-nematic phase is large at constant density in comparison to its stability range at constant pressure.
- (2) For a fixed value of x_0 and interaction parameter with given pressure, it is found that the number of nearest-neighbours γ influences the various thermodynamic properties. As γ increases the values of transition temperature, transition volume v^* , long range order parameter, entropy change and $dT_{N_D I}/dp$ increase, whereas the short range order parameter and Γ decrease.
- (3) For a given x_0 and interaction parameters, as the pressure increases the phase transition shifts to higher temperature, and both the fractional volume change $\Delta v/v$ and transition volume v^* decrease. A decrease in the values of the transition entropy and $dT_{N_D I}/dp$ is found, whereas the parameter Γ increases slightly.
- (4) At a given pressure, with decreasing value of the interaction ratio C_i/C_a and fixed C_i , the values of transition temperature, transition volume, fractional volume change, transition entropy, order parameters and $dT_{N_D I}/dp$ decrease and the parameter Γ increases.

Among extensive work [8, 10–12] on the phase transition in ordinary nematics and discotic-nematics, Somoza and Tarazona have developed a free energy density function theory (DFT) for the transition in various phases in the cases of parallel hard spherocylinders (PHSC) and parallel oblique cylinders. Their free energy of the real system is written in terms of that of parallel hard ellipsoids (PHE, as a reference system) with a correction factor in terms of the averaged Mayer function of the real system. The model has been used successfully to describe the nematic to smectic A phase transition both for PHSC and for a system of hard spherocylinders with free orientation. Somoza and Tarazona also obtained a first order transition between SmA and the columnar phase, in good agreement with computer simulation results [10]. Their various results are compared with computer simulation for larger molecular shape parameters (length-to-width ratio: 4 to ∞). Veerman and Frenkel [13] reported a computer simulation study of a system of 'hard cut spheres', oblate particles which serve as a model for disc-like mesogens.

The phase behaviour of this system is found to be strongly dependent on the length-to-width ratio of the particles, as in our results. In recent work, Averyanov reported [14] experimental data on the temperature dependence of the long range orientational order parameter in a discotic-nematic liquid crystal. He showed that the value of the orientational order parameter in the N_D phase is approximately the same as that of ordinary nematic liquid crystals. But the report did not predict the jump of order parameter at the transition temperature of the discotic-nematic to isotropic transition. Our results present the value of both types of order parameters at the transition point. So we are not in a position to compare our results with Averyanov's experimental data.

In conclusion, the calculation demonstrates that the short range orientational order has a strong influence on the N_D –I transition properties. One remarkable finding is that both calamatic and discotic mesogens exhibit quite similar behaviours of their transition properties.

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