Prediction of the density-pressure-temperature behavior of the ebba liquid crystal, at the isotropic-nematic phase transition

Previsão do comportamento da densidade-pressão-temperatura do cristal líquido do ebba, na transição de fase isotrópica-nemática

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ABSTRACT

In this work, we have analyzed of density-pressure-temperature behavior of the EBBA liquid crystal at 1 atm by using first-order perturbation theory for Convex Peg HERSW model. We predicted quantitatively the experimental density-temperature behavior in this region of the diagram phase with $k = 3.7$ and $k' = 2.065$, and with $k = 3.8$ and $k' = 2.121$.

Keywords: Phase Transitions, Isotropic-Nematic, EBBA, Liquid Crystal.**RESUMO**

Neste trabalho, analisámos o comportamento de densidade-pressão-temperatura do cristal líquido EBBA a 1 atm, utilizando a teoria de perturbação de primeira ordem para o modelo Convex Peg HERSW. Previmos quantitativamente o comportamento experimental da densidade-temperatura nesta região da fase do diagrama com $k=3,7$ e $k'=2,065$, e com $k=3,8$ e $k'=2,121$.

Palavras-chave: Transições de Fase, Isotropic-Nematic, EBBA, Cristal Líquido.**1 INTRODUCCION**

The main objective of any researcher is to generate or predict the qualitative and/or quantitative experimental behavior of some phenomenon (model or real system) present in nature. For this, they have had to establish theoretical models that allow making inferences about this phenomenon, for example, generate an analytic theory or perform computer simulations (Allen & Tildesley, 1991).

Apart from developing theoretical models, it is necessary to evaluate the prediction capacity, that is, to carry out the validation of the theoretical model to compare the results with experimental data of the real model (Cervantes et al., 2017). However, when a theoretical model is generated, in most cases, the study is limited only to describe the qualitative behavior and, partially, the quantitative behavior of the phenomenon. The causes why this can occur, could be that the researcher, in his academic training, has not developed the research competence, which can be acquired by using and implementing methodologies to carry out a research work (Jaik, 2013). A particular example of this is presented in studies where the objective is the prediction of the thermodynamic behavior, in the phase

transitions of the Liquid Crystals (Allen, 1995), which are intermediate states of matter (mesophases) between the Isotropic liquids and crystalline solids. Liquid Crystals present fluidity, that it allows them to occupy the shape of the container in which they are stored (also they present birefringence). Although in the literature some researchers reported data of experimental measurements (for example, the density-pressure-temperature behavior in the Isotropic-Nematic (I-N) phase transition (Kuss, 1978; Van Hecke, 2001), which, through a process of adjustment, state equations are generated) which are essential to carry out the validation of the theoretical models (in most cases it is not carried out). For this reason, in the present work, the validation process of a theoretical model will be carried out, implementing the MEPPS methodology (Cervantes et al., 2017) to predict of experimental behavior density-pressure-temperature of the Liquid Crystal EBBA [N-(p-Ethoxy-Benzylidene) p-n—Butyl-Aniline] at 1 atm.

2 CONCEPT OR PRE-PRODUCTION

EBBA is a Liquid Crystals (LC's), can be used as a lubricant because it reduces friction between surfaces (Cognard, 1989), since the low friction coefficients and a smaller viscosity value are maintained in the Nematic phase (N) compared to the Isotropic one (I), even when the temperature increases and the I-N phase transition is exceeded. This occurs because the I-N phase transition depends on the pressure and variations of density. For this reason, it is necessary to have a broad knowledge, from the theoretical and experimental point of view, of the density-temperature behavior in the Isotropic-Nematic phase transition (I-N) of the EBBA to 1 atm.

3 ANALYSIS

At this stage, experimental data were searched in the literature to be used in the validation process of the theoretical model. In Table I and II are reported the density-pressure-temperature experimental data (Kuss, 1978; Van Hecke, 2001; Muhoray P. & Balzarini, 1981), to calibrate the model by comparison with the theoretical results, where $T \equiv T_{Tr} \equiv T_{IN}$ is the triple point temperature or I-N phase transition temperature, $P \equiv P_{Tr} \equiv P_{IN}$ is the triple point pressure or I-N phase

transition pressure, ρ_I and ρ_N are I and N densities in the triple point pressure or I-N phase transition, respectively.

The phase diagram presents a Vapor-Liquid coexistence (V-L) that ends in a critical point T_c , a Vapor-Liquid-Nematic triple point (V-L-N) below which the N phase coexists with the phase of Vapor (V). Between the triple point and the critical point, the N phase coexists with the Liquid phase (L) and above the critical point with a supercritical Isotropic Fluid.

Table I. Pressure-Temperature and Density behavior in the I-N Phase transition for EBBA.

T_{IN}/K	P_{IN}/bar	$\rho_I/g \cdot cm^{-3}$	$\rho_N/g \cdot cm^{-3}$
351.9	1	0.9820	0.9841
355.5	100		
362.9	300		
370.0	500		
376.9	700		
383.4	900		
389.8	1100		
396.0	1300		
401.9	1500		
407.6	1700		
412.8	1900		
418.1	2100		

Table II. The Density [$\rho/g \cdot cm^{-3}$] in the Isotropic and Nematic Phase as function of Pressure.

P_{IN}/bar	80 °C	90 °C	100 °C	110 °C	120 °C	130 °C
1	<u>0.9881</u>	0.9803	0.9726	0.9649	0.9572	0.9490
100	0.9972	0.9865	0.9790	0.9715	0.9639	0.9558
200	1.0034	<u>0.9927</u>	0.9853	0.9780	0.9706	0.9624
300	1.0094	1.0015	0.9914	0.9843	0.9767	0.9689
400	1.0153	1.0077	0.9975	0.9905	0.9830	0.9750
500	1.0208	1.0136	<u>1.0034</u>	0.9964	0.9891	0.9807
600	1.0260	1.0192	1.0119	1.0024	0.9946	0.9867
700	1.0309	1.0245	1.0176	1.0079	1.0005	0.9924
800	1.0356	1.0296	1.0231	<u>1.0134</u>	1.0060	0.9980
900	1.0402	1.0344	1.0281	1.0210	1.0113	1.0034
1000	1.0446	1.0390	1.0331	1.0261	1.0164	1.0085
1100	1.0488	1.0433	1.0378	1.0311	<u>1.0211</u>	1.0134
1200	1.0529	1.0475	1.0422	1.0360	1.0285	1.0183
1300	1.0569	1.0516	1.0464	1.0403	1.0331	1.0228
1400	1.0608	1.0556	1.0506	1.0446	1.0376	<u>1.0275</u>
1500	1.0645	1.0595	1.0541	1.0484	1.0418	1.0345

In order to identify the range of validity of the theoretical model, it is necessary to consider the limitations that may have the theoretical model, for example the existence of ordered phases, such as a Liquid-Vapor-Smectic triple point (L-V-Sm) or Liquid-Vapor-Crystalline Solid triple point, which can occur, since

the triple point, for the I-N phase transition occurs at a pressure equal to zero, which would be very close to the triple points L-V-Sm and L-V-K. However, here it is important to mention that EBBA experimentally does not present these behaviors (Van Hecke, 2001).

4 DESIGN

The non-formal model, utilized in this paper, is expressed by a first-order Baker-Henderson type perturbation theory for the HERSW Convex Peg model (García-Sánchez et al., 2000), in which, the N molecules in a volume V at a temperature T are characterized by a hard uniaxial ellipsoidal core (HER) surrounded by a square well (SW) which is close to the edge of the hard core at the end of its major axis. The expression for the Helmholtz free-energy is given by:

$$\frac{A}{Nk_B T} = \frac{A_{ideal}}{Nk_B T} + \frac{A_{\Omega}}{Nk_B T} + \frac{A_{excess}}{Nk_B T} + \frac{A_{attractive}}{Nk_B T}, \quad (1)$$

where k_B is the Boltzmann's constant, A_{ideal} is the ideal contribution to the free energy, A_{Ω} is a contribution to the free energy coming from the loss of entropy due to the orientational order, A_{excess} is the free energy of the reference fluid and $A_{attractive}$ is the attractive contribution of free energy, the ideal contribution is given by

$$\frac{A_{ideal}}{Nk_B T} = \ln(N\Delta^3/V) - 1, \quad (2)$$

Where Δ is the De Broglie's mean thermal wavelength. The orientational term of free energy is given by the Onsager's expression (Onsager, 1949).

$$\frac{A_{\Omega}}{Nk_B T} = \int f(\Omega) \ln[4\pi f(\Omega)] d\Omega \quad (3)$$

where $f(\Omega)$ is the one particle orientational distribution function for a solid angle Ω , in the I phase $f(\Omega)$ is uniform, whereas for a N phase $f(\Omega)$ is a no uniform function. The hard core or excess free energy is given by:

$$\frac{A_{excess}}{Nk_B T} = \frac{\langle V_{excl}^{HC}(\Omega_1, \Omega_2) \rangle_{\Omega_1, \Omega_2}}{8V_0} \left[\frac{4\eta - 3\eta^2}{(1-\eta)^2} \right], \quad (4)$$

where $V_0 = V_{HS}$ is the volume of the Hard Sphere core, $\eta = NV_m/V$ is the packing fraction, V_m is the molecular volume, $V_{excl}^{HC}(r_{12}, \Omega_1, \Omega_2)$ is the excluded volume generated by the interaction between hard cores of two particles with orientation Ω_1 and Ω_2 , the angular brackets represent a weighted average over the molecular orientations. The attractive contribution to the free energy is given by:

$$\frac{A_{attractive}}{Nk_B T} = -4\eta \left(e^{\frac{1}{T^*}} - 1 \right) \left[\left(\frac{b_\lambda}{b} \right)^2 \frac{\langle V_{excl}^{atr}(\Omega_1, \Omega_2) \rangle_{\Omega_1, \Omega_2}}{8V_0} - \frac{\langle V_{excl}^{HC}(\Omega_1, \Omega_2) \rangle_{\Omega_1, \Omega_2}}{8V_0} \right], \quad (5)$$

where $T^* = \frac{K_B T}{\varepsilon}$ is the reduced temperature, $\frac{V_m^{atr}}{V_m^{HC}} = \left(\frac{b_\lambda}{b} \right)^2$, V_m^{HC} is the molecular volume of the hard core region, V_m^{atr} is the molecular volume of the attractive core region, b is the semi-minor axes of the hard uniaxial ellipsoidal core, b_λ is the semi-minor axes of the attractive ellipsoidal core, $V_{excl}^{atr}(r_{12}, \Omega_1, \Omega_2)$, is the excluded volume generated by the interaction between the attractive core of a particle with an orientation Ω_2 , and the attractive core of another particle oriented around Ω_1 . In general

$$\frac{\langle V_{excl}(\Omega_1, \Omega_2) \rangle_{\Omega_1, \Omega_2}}{8V_m} = d_0(k) - 16\pi^2 \sum_{n=1}^4 d_n(k) \left[\int_0^1 P_n(x) f(x) dx \right]^2 \quad (6)$$

where, for the case of the excluded volume, $x = \cos \theta$, $dx = -\sin \theta d\theta$, $P_n(\cos \theta) = P_n(x)$ are the even Legendre polynomials, and finally, the even values for $d_n(k)$ are presents in Table III.

Table III. $d_n(k)$ for the excluded volume between two ellipsoids.

$d_0(k)$	1.0404224126634527- 0.2124822065050437911k+0.200376367800779497k ² - 0.0452960284393375545k ³ +0.00574306142400010699k ⁴ - 0.000379115304850269341k ⁵ +0.0000101212234726092131k ⁶
$d_2(k)$	0.0179333444346647663- 0.181480728982367889k+0.19209470067370038k ² - 0.047788875213772485k ³ +0.00632342440673977534k ⁴ - 0.00042675267423366616k ⁵ +0.0000101212234726092131k ⁶
$d_4(k)$	0.0194078111400190493- 0.0239566112411885301k+0.00203625455229150542k ² +0.00598992119559058089k ³ -0.00180995207304058407k ⁴ +0.00024059689272044018k ⁵ -0.0000222110948667727814k ⁶ +0.00000100621182481881099k ⁷
$d_6(k)$	-0.010292896516519108+0.0245974193467313462k- 0.022282083144730383k ² +0.00958219741464688645k ³ -0.00210026578555277954k ⁴ +0.000276712894861745617k ⁵ -0.000022211094866727814k ⁶ +0.00000100621182481881099k ⁷ - 0.0000000197936446851484646k ⁸
$d_8(k)$	0.00340145568249058971- 0.0103737138719856858k+0.0128603133989782225k ² -0.00834614249029559651k ³ +0.00306427700897882848k ⁴ - 0.00065850083307786612k ⁵ +0.0000871812524289356005k ⁶ - 0.00000703189845731186569k ⁷ +0.000000317576022608253305k ⁸ - 0.0000000061611627577897798k ⁹

The state, input, intern, and output parameters and variables of the non-formal model are described in Table IV, as well as their respective restrictions.

The pressure and chemical potential reduced can be determined by the next equations:

$$P^* = \frac{PV_m}{k_B T} = \eta \left[1 + \eta \left(\frac{\partial(A-A^{ideal})}{\partial \eta} \right) \right] \quad (7)$$

$$\mu^* = \frac{\mu}{k_B T} = \ln(\eta) + \left(\frac{A-A^{ideal}}{N k_B T} \right) + \eta \left(\frac{\partial(A-A^{ideal})}{\partial \eta} \right) \quad (8)$$

In order to obtain the non-formal model values that would predict the density-pressure-temperature behavior in the I-N phase transition of LC EBBA, it is necessary to perform a minimization process of the Helmholtz free energy functional, for which it is used the test function method, since Helmholtz free energy functional depends on $f(\Omega)$. This process consists of (Figure 1):

- Select and substitute the input parameters T^* , b_λ/b , k and k' in the Helmholtz free energy functional expression.
- Helmholtz free energy in N phase, is obtained by replacing and evaluating the (Onsager, 1949) test function $f(\Omega) = [\alpha \cosh(\alpha \cos \theta)/4\pi \sinh \alpha]$ in equation (1), and performing the respective operations. After that, it is followed the minimization process for internal parameter α , which consists in minimizing the free energy over a wide atomic packing factors range of values. The minimized values for the internal parameter are adjusted for a polynomial in function of the atomic packing factor and then, the values are replaced again in the free energy functional obtaining the minimized free energy for the Nematic phase.
- The Helmholtz free energy in I phase, is obtained by replacing and evaluating $f(\Omega) = 1/4\pi$ in equation (1) and performing the respective operations.
- The pressure and chemical potential expressions for each phase (I and N), are obtained using equations (7) and (8).
- To determine the behavior in the I-N phase transition, the equilibrium condition is applied, which implies that chemical potential ($\mu_N^* = \mu_I^*$) and pressure ($p_N^* = p_I^*$) are equal respectively.

Table IV. Non-formal model parameters and variables with their characteristics

Parameter	Name	Type	Constraints	Units
A	Helmholtz free energy			J
A^{id}	Ideal Helmholtz free energy			J

N	Number of molecules		$(0, \infty)$	
k_B	Boltzmann constant	constant	$1.38064852 \times 10^{-23}$	J/K
$T^* = k_B T / \varepsilon$	Reduced temperature	input	$(0, \infty)$	
T	Temperature	state	$(0, \infty)$	K
P	Pressure	state	$[0, \infty)$	Bar
P_I^*	Reduced Pressure I	output	$[0, \infty)$	
P_N^*	Reduced Pressure N	output	$[0, \infty)$	
ρ	Density	state		
μ	Chemical potential	state		
μ_I^*	Chemical potential I	output		
μ_N^*	Chemical potential N	output		
ε	Depth of square well		$(0, \infty)$	J
$\eta = NV_m/V$	Atomic packing factor		$[0, 1]$	
V	System volume	state	$(0, \infty)$	m^3
V_m	Molecular volume		$(0, \infty)$	m^3
V_m^{HC}	Hard core molecular volume		$(0, \infty)$	m^3
η_I	Atomic packing factor I	output	$[0, 1]$	
η_N	Atomic packing factor N	output	$[0, 1]$	
V_m^{atr}	Attractive core molecular volume		$V_m^{atr} > V_m^{HC}$	m^3
$k = a_p/b$	Hard ellipsoid principal axis to semi-axis ratio	input	$[3, 10]$	
b y c	Hard ellipsoid semi-axes		$b = c$	
a_p	Hard ellipsoid principal axis		$a_p > b$	
$k' = a_p/b_\lambda$	Attractive ellipsoid principal axis to semi-axis ratio	input	$[3, 10]$	
b_λ y c_λ	Attractive ellipsoid semi-axes		$b_\lambda = c_\lambda$	
b_λ/b	Hard core semi-axis to attractive core semi-axis ratio	input	$\frac{b_\lambda}{b} = \sqrt{\frac{V_m^{atr}}{V_m^{HC}}}$	
α	Variational parameter	intern

Figure 1. Flow diagram for the Helmholtz free energy minimization process.

5 DEVELOPMENT

In Table V (García-Sánchez et al., 2015), are presented several external values of variables and parameters from the theoretical model that cannot be directly calculated, and that are crucial to carry out the experimental data comparison.

Table V. Theoretical parameters required to predict the experimental behavior for EBBA.

$V_m^{HC}/\text{\AA}^3$	$V_m^{atr}/\text{\AA}^3$	k	k'	b_λ/b
94.55	305.84	3.0	1.668	1.799

For the implementation stage, initially the program code is generated, based on the theoretical model by following a flow diagram. Nevertheless, it is important to notice that during the process syntax mistakes, non-valid processes, etc. are made, although they are detected in the validation and verification stage, when applying the MEPPS methodology (Cervantes et al., 2017), the process is returned of the implementation stage to carry out the debugging of the program and correct the errors detected, obtaining the final program of the theoretical model.

In Table VI, the theoretical model obtained data are shown for $k = 3.0$, $k' = 1.668$ and $b_\lambda/b = 1.799$.

Table VI. Obtained parameters using the theoretical model for the phase transition I-N for EBBA.

T^*	η_I	η_N	P^*
1	0.540528	0.558910	8.45003
0.9	0.522051	0.535220	6.07042
0.8	0.511368	0.526837	4.31868
0.7	0.494410	0.515083	1.95725
0.64	0.478125	0.506592	0.147322
0.635	0.476408	0.505910	0

To determine the prediction capacity for the theoretical model, it is necessary to calculate the square well value depth $\varepsilon = \varepsilon_{IN}$ using $T^* = \frac{K_B T}{\varepsilon}$ in the triple point ($T^* \equiv T_{Tr}^* \equiv T_{IN}^*$) with the experimental value 351.95 K for EBBA at this point (Van Hecke, 2001), we obtained that $\varepsilon_{IN} = 7.673361822 \times 10^{-21} J$, setting this value, the other temperature values would be determined by $T = T^* \varepsilon_{IN} / K_B$. To calculate pressure, it is used $P = P_i + \varepsilon T^* P^* / V_m = P_i + \varepsilon_{IN} T^* P^* / V_m^{HC}$ (where $P_i = 1 \text{ atm}$) and to determine density it is used $\rho = \frac{M_r \eta}{N_A V_m}$, where N_A is Avogadro constant (6.022×10^{23} molecules/mol) and M_r is the molar mass or relative molecular mass (281.39 g/mol for EBBA). To determine density in I phase $\rho_I = \frac{M_r \eta_I}{N_A V_m}$ and for N phase $\rho_N = \frac{M_r \eta_N}{N_A V_m}$ are used. Respecting to pressure-temperature behavior in the phase diagram region, described by phase transition I-N, the theoretical model predicts quantitatively (see figure 2).

Figure 2. Comparison between the theoretical prediction (line with asterisks) and the experimental data (solid line) of pressure-temperature behavior in the I-N phase transition for EBBA at 1 atm (Van Hecke, 2001).

Respecting to the experimental behavior for density-temperature in the triple point behavior in the I-N phase transition, it can be observed in Table VII, that the theoretical model cannot predict quantitatively this experimental behavior.

Table VII. Pressure-Temperature (Van Hecke, 2001). and Density (Muhoray P. & Balzarini, 1981) in the triple point for EBBA.

	Experiment	In this work
T_{IN}/K	351.9	351.9
P_{IN}/bar	1	1
$\rho_I / g \cdot cm^{-3}$	0.9820	2.3544
$\rho_N / g \cdot cm^{-3}$	0.9841	2.5002

It is possible to note that for EBBA the density-pressure-temperature experimental behavior is not predicted quantitatively. This may occur due to two situations, the first one is because no experimental values of the density were used in the triple point of the I-N phase transition. The second one arises due to that the molecular volume depends directly on the density. However, it is important to comment that, if this parameter is modified then, the theoretical model is unable to predict quantitatively the pressure-temperature experimental behavior in the I-N phase transition, since the value of the pressure depends on the molecular volume.

To solve this situation, and considering that Parsons proposed the following expression, which allows to relate to I-N phase transition temperature, molar

volume and intermolecular potential through the γ parameter (Parsons, 1979),

$$\frac{k_B T_c}{\varepsilon} = \left(\frac{\eta}{\eta_c^*} \right)^\gamma, \quad (9)$$

where T_c defines a critical temperature, which is the I-N phase transition temperature and η_c^* is the critical reduced packing fraction. In this work, we propose that γ be a parameter that allows to relate to temperature, molecular volume, packing fraction, density and intermolecular potential. On the one hand, we propose that γ be a parameter that allows varying the depth of the square-well potential, without modifying the intermolecular potential, though $\varepsilon = \gamma_{IN} \varepsilon_{IN} = \gamma_I \varepsilon_I = \gamma_N \varepsilon_N$, where $\gamma_{IN} = 1$ in the triple point for I-N phase transition, ε_I and ε_N are the potential square well depths in the phases I and N respectively, γ_I and γ_N are fitting parameters for I phase and N phase, respectively, and on the other hand, that $V_m = \gamma_{IN} V_m^{HC} = \gamma_I V_m^{HC} = \gamma_N V_m^{HC}$.

The adjustment parameters that were utilized to predict the pressure-density-temperature experimental behavior in phase transition I-N for EBBA at 1 atm are presented in Table VIII.

Table VIII. Parameters or variables required to predict the pressure-density-temperature behavior in the I-N transition phase for EBBA.

γ_{IN}	ε_{IN}/J	γ_I	ε_I/J	γ_N	ε_N/J
	6.6	2	2.823	2	2.578
	97×10^{-21}	.3718	6×10^{-21}	.5973	4×10^{-21}

Using the parameter values from Table VIII, the pressure-temperature behavior in the region of the phase diagram, described for I-N phase transition.

From the pressure-temperature experimental behavior, it can be observed that in region I, for $k = 3.7$ and $k' = 2.065$ (Figure 3) and $k = 3.8$ and $k' = 2.121$ (Figure 4) and in region N, $k = 3.7$ and $k' = 2.065$ (Figure 5) and $k = 3.8$ and $k' = 2.121$ (Figure 6), the theoretical model can predict quantitatively that experimental behavior.

Figure 3. Density-temperature plot for the theoretical model (asterisk line) and experimental data (solid line) in the region I of the phase transition I-N for EBBA with $k = 3.7$ and $k' = 2.065$.

Figure 4 Density-temperature plot for the theoretical model (asterisk line) and experimental data (solid line) in the region I of the phase transition I-N for EBBA with $k = 3.8$ and $k' = 2.121$.

Figure 5 Density-temperature plot for the theoretical model (asterisk line) and experimental data (solid line) in the region N of the phase transition I-N for EBBA with $k = 3.7$ y $k' = 2.065$.

Figure 6. Density-temperature plot for the theoretical model (asterisk line) and experimental data (solid line) in the region N of the phase transition I-N for EBBA with $k = 3.8$ y $k' = 2.121$.

6 RESULTS INTERPRETATION

It was demonstrated that the density-pressure-temperature experimental behavior in the phase transition I-N, is consistent with the obtained results in this work.

- As in the system it is shown a temperature increase, the molecules start its kinetic energy, which allows the molecules to overcome the short range attraction forces, resulting that molecules start to collide causing a pressure increase.

- It is observed that density in N Phase is larger than in I phase, since molecules in N phase are oriented, they can move and be agglomerated more easily, unlike I phase, with the consequence of in N phase, viscosity is smaller than in I phase.

- As a consequence of the equilibrium between both phases, it is found a larger molecule ordering in phase N with respect to I phase. This promotes an increase of pressure and temperature, which is compensated with small variations in density values for both phases.

- The theoretical model predicts quantitatively the density-pressure-temperature experimental behavior in the phase transition I-N.

Since the theoretical model predicts quantitatively the density-pressure-temperature experimental behavior in the I-N phase transition for EBBA at 1 atm, the computational program can be utilized to predict this behavior for other Liquid Crystals.

7 IX CONCLUSIONS AND PERSPECTIVES

In this work, we have analyzed the experimental density-pressure-temperature behavior of the I-N phase transition of the liquid crystal EBBA at 1 atm. We predicted quantitative the experimental density-pressure-temperature behavior in this region of the diagram phase with $k = 3.7$ and $k' = 2.065$, and with $k = 3.8$ and $k' = 2.121$.

Other important factors that might be modified in later studies to improve the theoretical prediction, would be to consider in the Helmholtz free energy expression the following: the model might be described by means of biaxial core, the incorporation of the flexibility and polarity effect, and the consideration of the large range interactions, since it is possible, as the molecule size increases, the contributions to the free energy from these parameters are more important.

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