Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl20

The Modeling with Free Boundary

M. E. Agelmenev [a]

[a] The Institute of Organic Synthesis and Chemistry of Coal of the Republic of Kazakhstan, Karaganda, Republic of Kazakhstan

Version of record first published: 30 Jun 2011

To cite this article: M. E. Agelmenev (2011): The Modeling with Free Boundary, Molecular Crystals and Liquid Crystals, 545:1, 190/[1414]-203/[1427]

To link to this article: http://dx.doi.org/10.1080/15421406.2011.572010

Mol. Cryst. Liq. Cryst., Vol. 545: pp. 190/[1414]–203/[1427], 2011

ISSN: 1542-1406 print/1563-5287 online
DOI: 10.1080/15421406.2011.572010

The Modeling with Free Boundary

M. E. AGELMENEV

The Institute of Organic Synthesis and Chemistry of Coal of the Republic of Kazakhstan, Karaganda, Republic of Kazakhstan

In this work the results of modeling of the liquid crystals that have different types of the mesomorphism are presented. The simulation was done by the method of the molecular dynamics without setting boundary conditions, which is allowed for recording the liquid aggregate state.

Keywords Arylpropargyl ethers of phenols; asymmetrically substituted 1,1′-bis ferrocene; modeling with free boundary; nematic and smectic liquid crystal

1. Introduction

Computer modeling of processes with molecular dynamic and Monte-Carlo methods in different molecular systems faces two major problems: the search for a condition that requires less total energy and influence of the boundaries. The problem gets harder while analyzing liquid-crystal systems for which a presence of the long-range orientational order is typical. In this case, using periodical boundary conditions is not fully correct. As it was shown in many works [1–5], to achieve the minimum level of the system's energy the required simulation time must vary in a wide range, between 650 ps and 40 ns. These values restrict the number of molecules and conditions that can be used. Consequently, it is hard to obtain from *ab initio* simulations a precise information about possible temperature ranges of phase transitions for compounds that have not yet been synthesized.

Is the equilibrium condition obtained by a minimization of the system's energy by means of the *ab initio* and quantum-chemical methods indisputable? As it was shown in [6,7], the structure of molecules in crystalline form (x-ray analysis) and gas form (*ab initio* and quantum-chemical methods) differs from each other. Considering that boundaries set their own corrections on the dynamical behavior of a cluster, it is necessary to state that an answer to the question above can be problematic. Therefore we need to consider which state of aggregation of matter is necessary during the modeling. It is especially important for liquid crystals.

As it is shown in the [8,9], at the big modeling times without setting the boundaries the ordering degree of the liquid crystals tends to vanish. Obviously, this fact contradicts with real physical nature of the researched compounds. Therefore, in

Address correspondence to M. E. Agelmenev, The Institute of Organic Synthesis and Chemistry of Coal of the Republic of Kazakhstan, 100000, Karaganda, Alikhanova Str., 1, Republic of Kazakhstan. Tel.: +7-7212-413866; Fax: +7-7212-413865; E-mail: amaxut@mail.ru

the given paper the results of modeling of various kinds of liquid crystals in the conditions of absence of boundaries and small times, in which orderliness is remained, is presented. The simulation was done by using method of molecular dynamic taking into account liquid aggregate state.

The choice of the modeling time was defined by conditions of a temperature influence and a condition of the sufficient fall of all cluster energy. The analysis of results [9] shows that average energy ΔH changes within 1 kcal/mol in an interval from 10 to 850 ps. It is comparable difference between conformations.

2. Experimental Methods

For the carrying out the behavior modeling of these compounds the set of programs under the general name GROMACS [10] version 3.3.1 has been used.

Methods of cluster formation and its researches were described in [9,11–12].

The presence of the ferrocene fragment in structure compound promotes development of the steady mesomorphism in many cases. In the work [13] one kind of such compound with asymmetrical replacement has been synthesized and investigated. The results of these researches show the difficult picture of phase transitions in the obtained compound and variety of the observable mesomorphism kinds.

For the purpose of finding-out of character of the processes proceeding at phase transitions in case of heating of such compound, experiments on computer modeling of their behavior have been made.

Gross-formula connection looked like $C_{63}H_{79}F_2FeNO$, consisting of 147 atoms. Considering that in [13] was not accurate data on geometry, we had been conducted researches of prospective structure in some stages. It has been connected with possibilities of the quantum-chemical methods limited in sizes of counted molecules. The fragment with participation of atom of iron and attached to it cycles has been investigated with the help of non empirical method GAMESS version 6.4. Molecule chains were optimized by half empirical method MNDO. Final optimization of geometry of all compounds with the account of charging conditions on atoms has been carried out by means of Gromacs software package. The initial structural data was set by results of the abovementioned calculations. The modeling time at last stage of definition of molecule geometry was equal to 5 nanoseconds (300 K). It is established that the total energy of the investigated molecule was equal to 1327.7 kJ/mol, where the contribution of the potential energy-781.1 kJ/mol and kinetic energy-546.6 kJ/mol. The final geometry of a molecule is presented on Figure 1.

In subsequent of the received molecules cluster has been constructed, where they settled down in parallel each other in conformity with the data of experimental researches [13].

At carrying out of computer modeling consecutive annealing has been done [11–12]. The size of the initial cluster had the following sizes $-10 \times 6 \times 11$ molecules

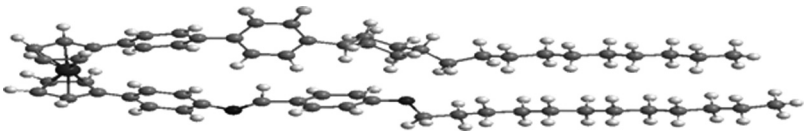

Figure 1. Geometry of the asymmetrically 1,1′-bis substituted ferrocene.

and included 660 molecules or 97020 atoms. At the construction of the initial cluster the long axis of a molecule has been directed along Y axis (direction of the director). Planes, in which molecules settled down, were parallel to OXZ plane.

Packing of the initial cluster had following parameters:

$X = 1.3$ nm (distance on x from the beginning of one molecule prior to the beginning of following); $Y = 3.4$ nm (distance on at from the beginning of one molecule prior to the beginning of following); $Z = 0.8$ nm (distance on z from the beginning of one molecule prior to the beginning of following); $\Delta X = \Delta Y = 0$ (without displacement).

The first layer of molecules (60 molecules = 8820 atoms) was considered motionless (substrate) and did not participate in modeling. Molecules have been focused planar and homeotropically in relation to the substrate.

As it has been established in [13], at heating phase transitions had the following order – Cr1 365 K Cr2 476 K Sm 489 K N 545 K I, where Cr1 and. Cr2 correspond to a crystalline state with presence of three and sets of layers, respectively, and Sm is a smectic C phase, N – a nematic phase, I – an isotropic liquid.

The annealing time at one temperature was 10 picoseconds, but at that condition cluster was settled down in one cell, so the liquid modular condition of the system has been realized [11,12]. The vector of intensity of electric field has been directed perpendicularly to the substrate, and its value was equal to 1.0×10^7 V/m.

3. Results and Discussion

3.1. *The Modeling of the Behavior of the Smectic Liquid Crystal at the Approach to the Liquid State*

The analysis of the modeling results has been done for two cases, when as directing molecules atomic pairs on both chains were chosen (Fig. 1). The qualitative picture of the received data has completely coincided. Therefore further results of the analysis will be shown for only one of the chosen directing.

The analysis of molecules distribution depending on the values of heat formation for detailed elaboration of the processes occurring at phase transitions has been carried out. The special program has been created for this purpose. Distribution of molecules according to heat formation from distance to the centre of cluster was corresponded to the total energy of all molecules which were in the given segment. The given distance corresponds to the large radius of the segment relative to the certain centre that was defined before. Also dependences of the average value of heat formation of one molecule in the given cluster segment have been defined. The centre of the cluster was defined by finding coordinates of the molecules that have maximum and minimum values.

The uniform energy distribution all along cluster, not including small deviations on border, has been established. It allows considering the condition of molecules in cluster close to equilibrium. The average values of heat formation of one molecule at the concrete temperature value in the basic part of cluster remain almost constant.

The results of experiments on computer modeling are presented in Figures 2–8.

The received results show good correspondence to the experimental data that is defined by inflection in the region of temperatures of phase transitions on curves of dependences of the ordering degree S(T) (Fig. 2), information entropy S_{inf} (T) (Fig. 2), volume of cell V (T) (Fig. 4), energy of the compound Eb (T) (Fig. 3),

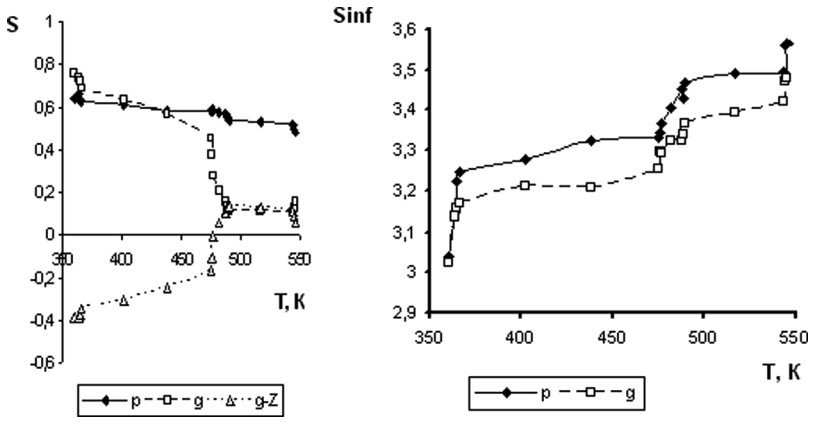

Figure 2. Temperature dependences of the ordering degree S(T) and the information entropy S_{inf} at planar (p) and homeotropical (g) subtract orientations.

number of molecules N (T) which longitudinal axes make an angle of 10° relative to the direction of the director (OY axis) (Fig. 3), functions of distribution D (T) of the molecules pairs which are located under a certain angle(Fig. 5). The D (T) plot is presented in polar coordinates, in the right part the axis of angle counting (from 0° to 90°) is the vertical axis, and in the left part – a horizontal axis (from 90° to 180°). The angle counting is made clockwise.

It can be seen from Figure 2 that the ordering degree in case of planar orientation keep high value (see the case **p**). At the homeotropical orientation after melting temperature that value start sharp decrease. It is caused by the turn of whole cluster relative to the substrate that proves by the g-Z, curve i.e., change of direction of the director.

As the S_{inf} (T) curves show (Fig. 2) the greatest order is observed at the homeotropical orientation. In many respects it is caused by possibility of the cluster expansion at the temperature influence along OZ axis.

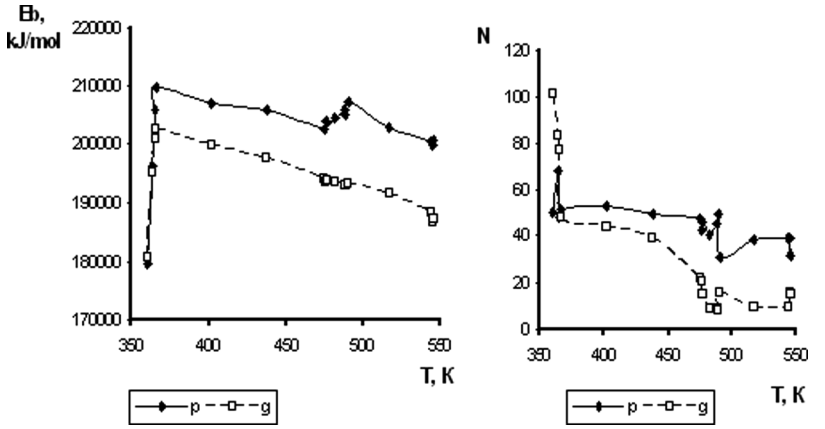

Figure 3. Temperature dependences of energy of the compound E_b and number of molecules N at planar (p) and homeotropical (g) subtract orientations.

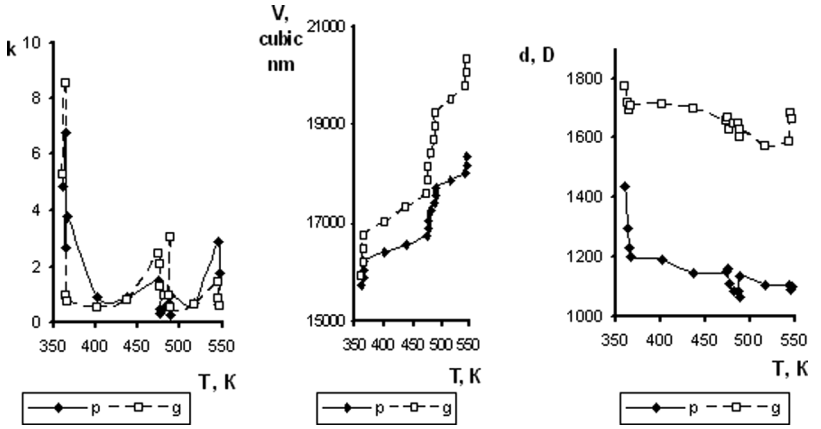

Figure 4. Temperature dependences of self-diffusion factor k ($[k] = nm^2/s$), volume of cell V and dipole moment d of cluster molecules at planar (p) and homeotropical (g) substrate orientations.

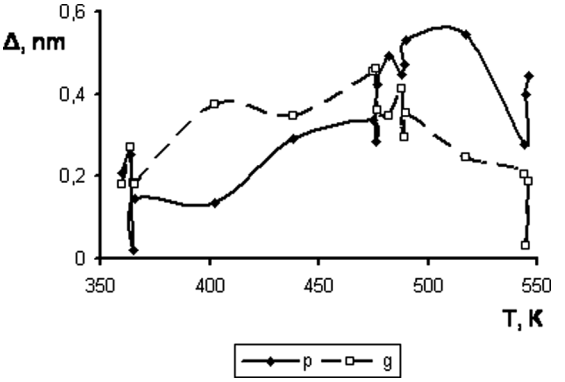

Figure 5. Temperature dependence of the displacement of adjacent molecules relative to each other, located at the centre of cluster.

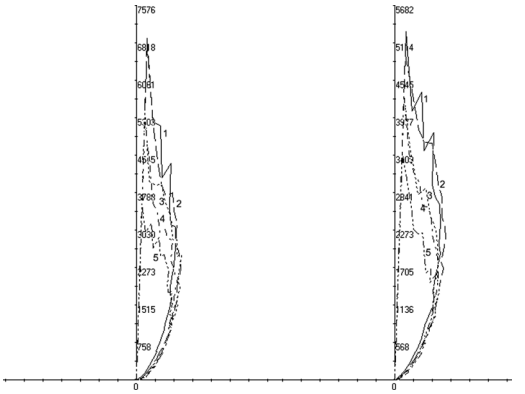

Figure 6. Distribution functions D of molecules' pairs in a crystalline state (1, 360 K), at temperatures of transition Cr1-Cr2 (2, 365 K), melting (3, 476 K), transition Sm-N (4, 489 K) and bleaching (5, 545 K) in case of planar (p) and homeotropical (g) orientations.

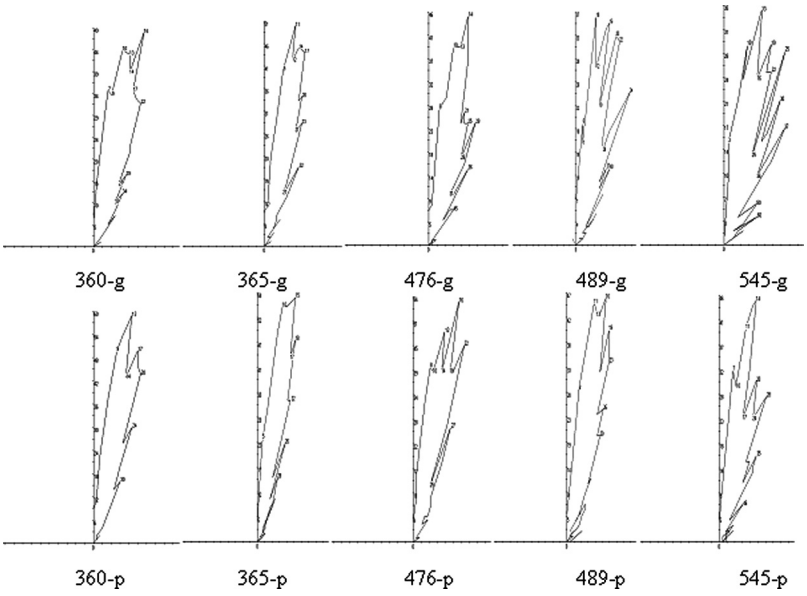

Figure 7. Distribution of molecules on angle between chains at various temperatures and substrate orientations.

Apparently, for the same reason at planar orientation higher values of compound energy Eb and N number are observed (see Fig. 3). In this case at the region of the smectic phase bond energy with temperature rise starts to increase. That is associated with the restrictions in displacement of molecules because of presence of the substrate perpendicular to the OZ axis. It leads to growth of heat formation of separate molecules. The absence of restriction at homeotropical orientation leads

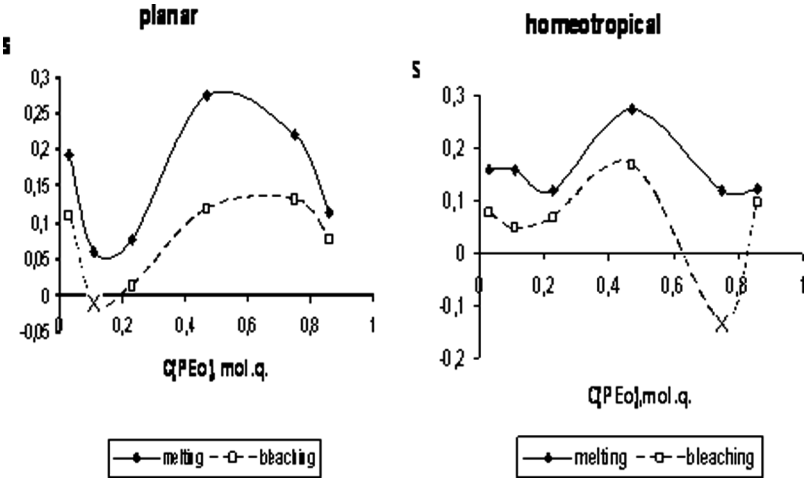

Figure 8. Dependence of the ordering degree at melting and bleaching on the mixture structure at various substrate orientations.

to increase in volume of cell V with the cluster in it (Fig. 4). The conservation of the high order causes the rise of the general cluster of dipole d molecules (Fig. 4).

The conservation of high order in many respects is caused by strong intermolecular interaction. The reason of it is the big sizes of investigated compound. Therefore, at temperature influences the mobility of such compounds will be small. The changes of self-diffusion coefficients k confirm observable tendencies for molecules next to the substrate and in the centre of cluster (Fig. 4).

The carried out analysis of the coordinates of the adjacent molecules, located in the centre of cluster, shows that with temperature rise the displacement Δ of the molecules relative to each other increase along all directions. Maximum displacement occurs along OZ axis. The displacement on the OY axis strongly increases especially at the transition from smectic phase to the nematic phase (Fig. 5).

It is matched with [14], that smectic phase is more ordered in comparison with nematic and the centers of gravity of molecules in it lie in one plane. The difference in the displacement change at hometropical orientation, most probably, is caused by strong movement at high temperatures of whole cluster relative to the substrate.

High asymmetric property of curves of the distribution function of pairs molecules D (α), located under defined angle to each other (Fig. 6), shows that in process of the annealing molecules are not developed strongly, keeping the direction of the director almost invariable. It is enough to compare situation with nematic liquid crystals [11,12], where there are always pairs with angles, bigger then 90°. The curves shown correspond to the temperatures, which conform to the various phase conditions.

Two crystalline states differ by different packing of molecules [13]. For Cr1 condition 3 layers with big sizes, for Cr2 with set of small sizes are typical. The visual analysis of the cluster type at temperatures of existence of these conditions has allowed finding out in the region of Cr1 existence accurate stratification on pile of clusters' molecules and from the moment of transition Cr1 – Cr2 the beginning of the processes of their associations. It can be seen from Figure 6 that the maximum quantity of pair molecules in these conditions almost does not vary.

The significant reduction of D (α) occurs at the further rise of temperature. At both orientations of the substrate features on curves are found out in the form of the peaks, that is located in the regions close to the values of angles – 2 (maximum), ~5, ~9, ~14, ~22 degrees. The analysis of D (α) function values (on Fig. 6, curves 1 for a case p and g) give following values – 6812 (p) and 5284 (g) at 2°, 5153 and 4388 at 5–6°, 4429 and 3797 at 9°, 3184 and 2746 at 14°, 1863 и1264 at 22-28° accordingly. It is easy to see that with increase of angle of the subsequent peak there is a reduction of quantity of pairs somewhere on a quarter from the previous value. Presence of peaks on all curves says that their nature is caused by the nature of the compound.

The most sensitive to external influences fragment of a molecule is ferrocene, where there is a rotation of both chains relative to the atom of iron at the expense of mobility of five member cycles. In fact, the angle between molecule chains varies in limits from 9° to 22° at both orientations of the substrate (Fig. 7).

Plots of distribution of molecules at the internal angle (Fig. 7) between chains are constructed in polar coordinates, where the angle is counted from the vertical axis, and the length of radius corresponds to quantity of molecules. It is easy to see that with increase in temperature the value molecules with the exceeding the

specified limit angles, starts to grow. However, generally the majority of molecules have angles between chains within 9–22°.

The comparison of the results on this distribution and distribution of pairs molecules D (α) allows assuming the connection between peaks on Figure 6 and maxima on Figure 7. Considering that molecules have been constructed in parallel relative to each other in the initial cluster and at all stages of temperature influence there was no pair with angle larger than 90°, it is possible to assume a contiguity of angles projections on plane OXZ in the specified interval of 9–22°.

Thus, the experimental results from computer modeling show the difference of the molecules geometry, which are located in cluster, from the molecules geometry that was obtained from the optimization of initial compound. It is established that molecules in cluster represent conformers with various values of angles in ferrocene fragment. It causes the variety of mesomorphism, which was observed experimentally. It is shown that transition from one crystalline phase in another is caused by strengthening the cooperatives of intermolecular interaction as a result of temperature rise.

3. 2. *Modeling of Behavior of the Binary Mixtures at the Approach to the Liquid State*

Nematic liquid crystals based on arylpropargyl ethers of phenols (APEP) offer promise for the improvement of the temperature characteristics of liquid crystalline devices [11,12]. The perfecting of the mesogenic properties of compounds cannot be accomplished without detailed information about processes in them.

As it has been experimentally established earlier (Table 1), at the ratio of 1:3 phenyl propargyl ether of o-nitrophenol (PEo) to phenyl propargyl ether of *p*-fluorine phenol (PEF), the temperature interval of mesophase existence was equal to 90°. At the same time for curve dependences of melting and bleaching temperatures, dielectric anisotropies on the mixture structure, the nonlinear dependence is typical (Table 1).

The methodology of clusters constructions, arrangement of molecules relative to coordinate axes is the same as in Section 1. As in Section 1, NPT ensemble was used during the modeling, time of the modeling at the given temperature was 10 ps, intensity of the electric field was 1.0×10^7 V/m. The substrate was represented as the bottom boundary of the initial cluster on the XOY plane. During the modeling it has been frozen. The radiuses of the cutoff of dispersive and coulomb interaction were 2 nm. The consecutive annealing has been accomplished.

For finding-out the reasons of such dependence, experiments on computer modeling of the mixture behavior depending on its structure have been made.

Table 1. Some results of the binary mixture research (PEo + PEF) (C(PEo) – ratio of PEo in the mixture)

	C(PEo), mol. q.					
Temperature, K	0.03	0.11	0.23	0.47	0.75	0.86
Melting	298	296	293	299	296	298
Bleaching	348	381	383	368	381	383

Table 2. Dimensions of the studied clusters at various substrate orientations (dy – displacement of neighboring molecules from each other; x, y, z – distance between molecules along corresponding axes)

C(PEo), (PEF/PEo)	Size, molecule	X [nm]	Y [nm]	dy [nm]	z [nm] planar (homeotropical) orientation
0.03 (25:1)	$13 \times 13 \times 18$	0.9	1.6	0.7	0.4 (0.5)
0.11 (7:1)	$14 \times 14 \times 16$	0.8	1.6	0.7	0.5 (0.5)
0.23 (3:1)	$14 \times 14 \times 16$	0.8	1.6	0.7	0.4 (0.4)
0.47 (1:1)	$14 \times 14 \times 16$	0.8	1.6	0.7	0.4 (0.4)
0.75 (1:3)	$14 \times 14 \times 16$	0.8	1.6	0.7	0.4 (0.4)
0.86 (1:7)	$14 \times 14 \times 16$	0.8	1.6	0.7	0.5 (0.5)

The basic characteristics of the studied clusters are specified in Table 2.

The strong intermolecular interaction in the mixture, caused both by the presence of nitro group in the orto-position, and by the presence of the fluorine atom in the para position, leads to big inertness of the mixture molecules. It is proved by the small values of self-diffusion coefficient, and by the flatness of the temperature dependency curves of the ordering degree.

It is necessary to mention that on the curves of temperature dependences of the ordering degree (Fig. 8), volume of cells, information entropy, energy of compound there are typical bends in the region of melting and bleaching temperatures.

As seen from the Figure 8, the ordering degree has the greatest value at the equal quantities of both components. The greatest values are observed at the planar orientation. Due to the high inertia of the molecules that show prosperity to aggregation at the homeotropical orientation, the turn of all molecules ensembles is observed. It leads to the appearance of the negative values of ordering degree. These cases are marked in the Figure 8 by crosses ($\times$). It is caused by the increase level of freedom along axis OZ at such orientation. Generally, the nonlinear character of the ordering degree change from the compound is observed, that corresponds with experimental data.

In the Figure 9, curves of the distribution of pairs molecules functions D (α) are presented at various phase conditions. The corresponding temperatures are specified in figure legends.

For all curves the high asymmetry of the right and left part of the graphs is typical. The practical absence of the left part shows that small quantity of pair molecules between which the angle was more than 90°. It shows high the ordering degree. The best scenario is observed at values with C(PEo) = 0.47 and 0.75. The further increase and reduction of PEo level leads to decrease in the ordering degree. However, at the minimum containing of PEo (with C(PEo) = 0.03) the ordering degree increase is observed. In these cases respectively great values of D (α) in comparison with other compounds are observed. With temperature raise the left parts of graphs D (α) increase, right – decrease. At some curves the common points of intersection in the right part of the graph, lying in the region of 50–60° are observed, which are slightly higher than the values that were observed earlier [11,12]. The influence of the substrate orientation is not so equivocal.

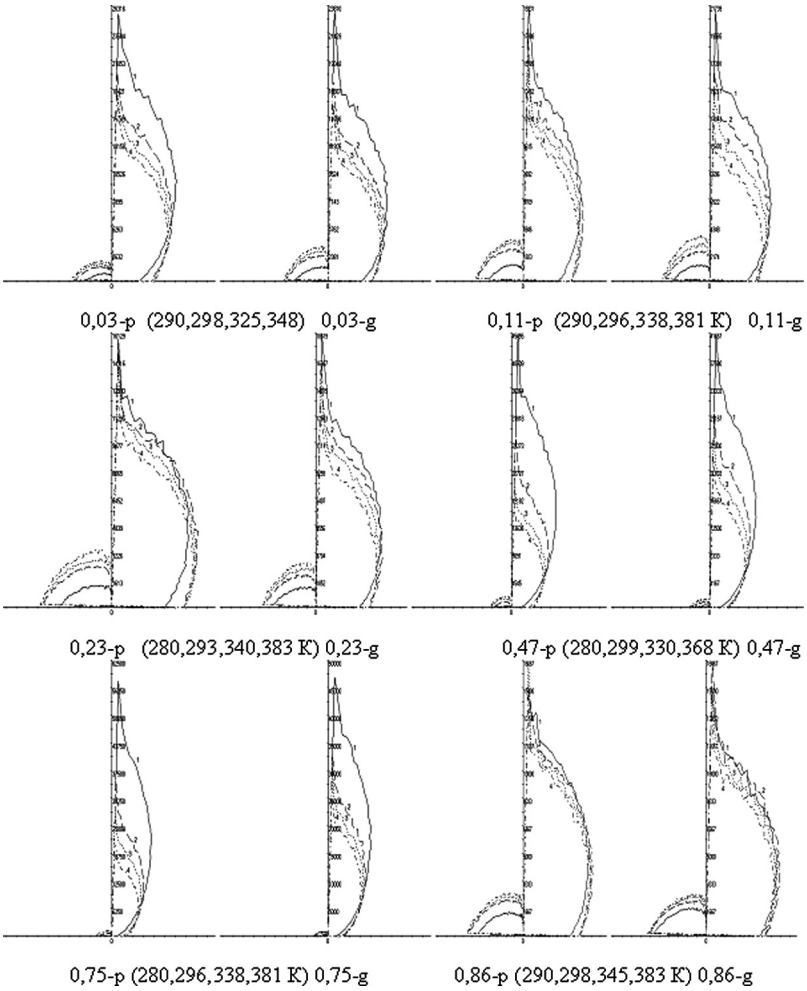

Figure 9. Distribution functions D of pair molecules at crystalline state (1), melting (2), mesophase (3) and bleaching (4) at various structures of the mixture and substrate orientations.

3.3. *The Determination of Possible Temperatures of Phase Transitions of Not Synthesized Nematic Liquid Crystals*

For approbation of the used approach, researches defining temperatures of phase transitions of hypothetical connection – *p*-nitro-phenyl property ether of phenol (Lap) were done, that as results of quantum-chemical calculation have shown [15] should have higher message in comparison with studied the APEP. The reason for such statement is the result of quantum-chemical researches about matching of directions of the dipole moment vector and the molecule longitudinal axis. The similar researches for p-nitro phenyl property ether of p-fluorine phenol (lpF) and p-nitro phenyl propargyl ether of p-chlorine phenol (lpCL) have shown that the direction of their vectors will have the angle with the longitudinal axis for about 20° It is essential smaller angles than that were observed on earlier investigated compounds [15], which are NLC with dielectric anisotropies of $\Delta\varepsilon < 1$. The small angles allow

expecting increase of the $\Delta\varepsilon$ in these compounds; therefore an increase of mesogen at such replacement. At the same time, polarity of nitro group and halogen atom, that are in para position, should promote their repulsion between each other, that will reduce the ordering and will decrease the melting temperature of such compounds.

Clusters had the size of $13 \times 13 \times 18$ molecules. The consecutive annealing was done. The searching of melting temperature was made by search through values of temperatures until achieving the moment of constancy of degree of orderliness values. After defining the melting temperature region, the values of annealing temperatures have been chosen and modeling of the behavior of all clusters was done, that were subjected to the sequent heating. The initial interval between the nearest temperatures was chosen as 5 degrees. Experiments were done at two orientations – planar (p) and homeotropical (g). The initial temperature has been chosen in the region of room temperature as the molecule structure is close to the structures of molecules investigated before in [12,16,17].

As can be seen from the Figure 10a, the curve of temperature dependence of the ordering degree of Lp at two orientations of the substrate has characteristic excessive bends. They allow to assume that possible value of melting temperature of this compound can lie in region of 283 K, bleaching -338 K. The error of -2° for melting region [11,12] is considered. The presence of clear excess bend in the region of the mesophase at 303 K allows assuming the existence of smectic phase, which is prior to nematic

As can be seen from the Figure 10a, the homeotropical orientation leads to ordering increase in comparison with the planar. It can be connected to the absence of the substrate in direction OZ that allows less breaking of the initial orderliness with temperature increase.

The detected points in the Figure 10a curves have a good compliance with the curve of information entropy temperature dependence (Fig. 10b).

The electric field presence does not lead to increase of the ordering degree at 320 K as it was observed for earlier researched polar APEP [11,12]. Apparently, it is connected with the best orderliness of this compound because of the compliance of directions of the dipole moment vector with the molecule longitudinal axis. It is finding the good compliance on curve temperature dependence of whole cluster dipole moment.

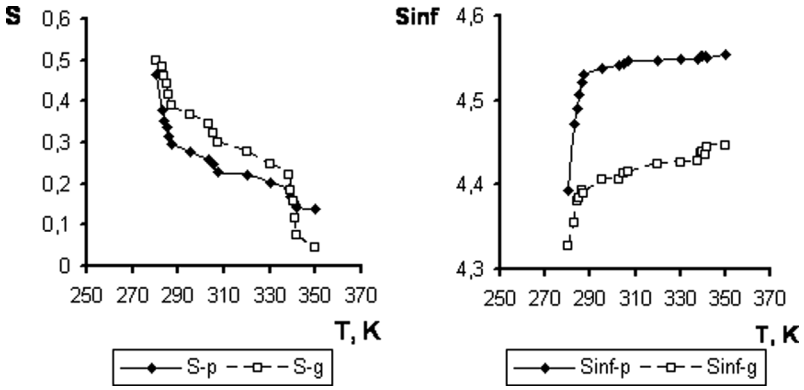

Figure 10. Temperature dependences of degree of orderliness (a) and information entropy (b) Lp at planar and homeotropical substrate orientations.

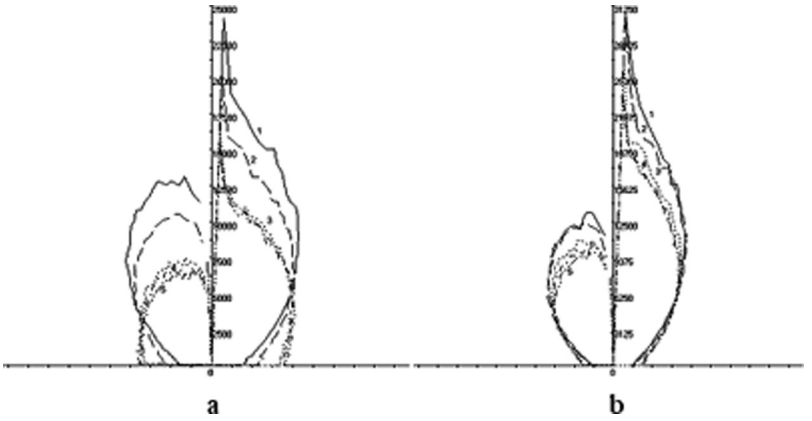

Figure 11. D (α) distribution functions of pairs of molecules at crystalline state (1, T = 280 K), at melting (2, T = 283 K), at phase transition from smectic to nematic condition (3, T = 303 K), at mesophase (4, T = 320 K), at bleaching (5, T = 338 K), at substrates planar (a) and homeotropical orientations (b).

As can be seen from the Figure 11, the enhancement of the ordering at homeotropical orientation is visible of how distribution function D (α) of quantities of pairs molecules, that are placed at the angle of α, changes. (Fig. 11b). There is no significant increase in pairs molecules at $\alpha = 90°$, as on the Figure 11a. The points of intersection of curves D (α) in the right and left part of the graph are: A – 45° and 125° and B – 40° and 130° respectively. The small difference between these values for two orientations probably can be connected with the general character of the given clusters' possible skeleton [11,12].

As can be seen from the Figure 12, on curves S (T) lpCL lpF compounds characteristic bends [11,12] are observed. They allow finding possible values of melting and bleaching temperatures. For the compound with chlorine (lpCl) atom they equal to

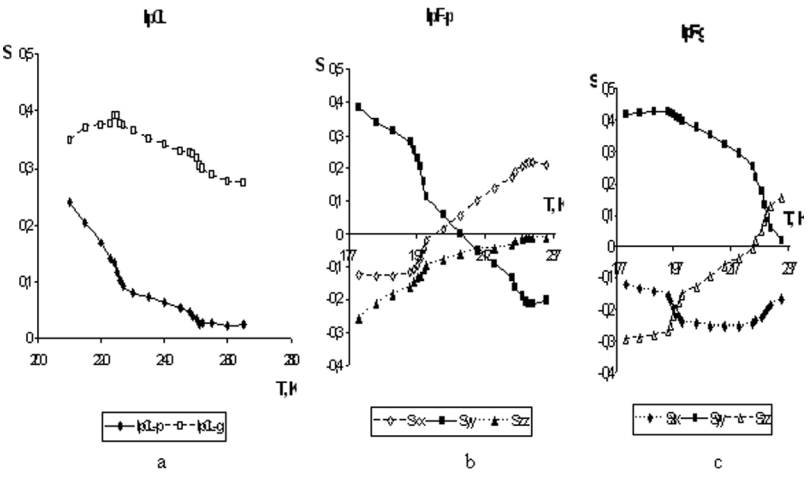

Figure 12. Temperature dependences of the ordering degree clusters, containing lpCL (a), lpF (b,c) molecules at planar (p) and homeotropical (g) substrate orientations.

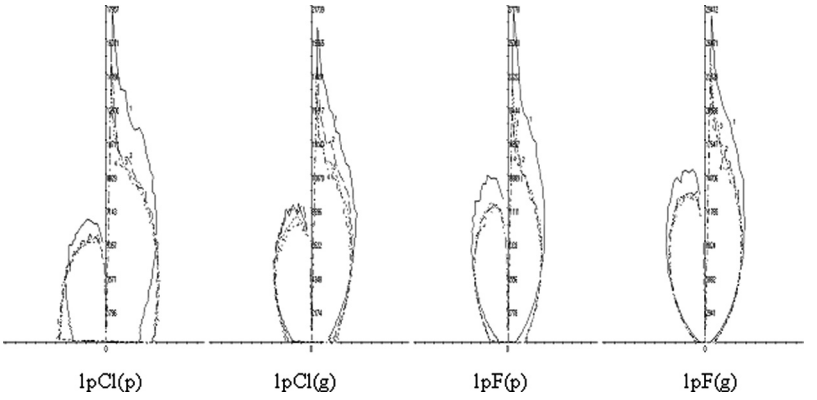

Figure 13. Temperature dependences of pair molecules distribution functions D (α) of clusters at various phase conditions and substrate orientations. lpCL – (1 – 210 K, 2 – 225 K, 3 – 235 K, 4 – 250 K), lpF – (1 – 180 K, 2 – 198 K, 3 – 205 K, 4 – 228 K).

225 K and 250 K respectively. At the same time, as it was observed earlier the homeotropical orientation promotes greater ordering.

As for molecules with atom of fluorine, (lpF) (Fig. 12b, 12c), it is necessary to mention the turn of molecules along OX axis at planar orientation of the substrate (Fig. 12b) and sharp decrease of the ordering regarding given direction of the director. The possible temperatures of phase transitions for lpF were 198 K and 228 K. Visual supervision shows that in this case the whole cluster is developed and only a small amount of its molecules are kept on the substrate. At homeotropical orientations such dramatic decrease of degree of ordering do not occur (Fig. 12c), and the turn of molecules occurs only at high temperatures, that lead to S_{zz} increase. Also at the homeotropical orientation in comparison with case of planar the ordering increase can be observed.

As can be seen from the Figure 13, the quantity of pair molecules, which are placed at the angle of 90^0, in clusters with lpF molecules is less in comparison with cluster with lpCL. The setting of homeotropical orientation for both molecules leads to the reduction of pair quantity, which is placed under this angle. The expressed asymmetry of curves shows good dynamics at temperature influence and high degree of ordering in the studied clusters [11,12]. The general points of intersection of curves for various phase conditions correspond to values of angles, which were observed in [11,12].

4. Conclusions and Perspectives

The temperature dependences received of the ordering degree, informational entropy, distribution function of pair molecules and other characteristics of molecules conditions in clusters do not contradict with experimental results. At the same time, the modeling under such circumstances allows creating big clusters and to consider features of molecules structure.

Undoubtedly, there are still questions on the achievement of condition of the cluster with least energy. However, application of physical and chemical understandings about the nature of mesomorphism at the cluster formation, the determination

of initial molecules structure by means of quantum-chemical methods, the setting of the substrate, the temperature and electric field influence essentially allows reducing the errors of such approach.

Acknowledgment

This work has been done in scope of the plan of the fundamental researches of the Ministry of Education and Science of the Republic of Kazakhstan.

References

[1] Wilson, Mark R. (2005). *Intern. Rev. in Phys. Chem.*, *24*, 421.
[2] Ilnytskyi, J. M., & Wilson, M. R. (2001). *J. Molecular Liquids*, *92*, 21.
[3] Berardi, R., Muccioli, L., & Zannoni, C. (2004). *ChemPhysChem*, *5*, 104.
[4] Care, C. M., & Cleaver, D. J. (2005). *Rep. Prog. Phys.*, *68*, 2665.
[5] Kai-Leung, Yung, Lan, He, Yan, Xua, & Jie, Kong. (2008). *Polymer*, *49*, 2770.
[6] Kitaygorodskii, A. I. (1971). *Molecular crystals* (in Russian), M.: Nauka.
[7] Bryan, R. F. (1982). *Zh. Strukt. Khim.*, *23*, 154.
[8] Wang, Zhiqiang, Lupo, James A., Patnaik, Soumya, & Pachter, Ruth. (2001). *Comput. and Theoret. Polymer Sci.*, *11*, 375.
[9] Agelmenev, M. E., Bratukhin, S. M., Muldakhmetov, Z. M., & Polikarpov, V. V. (2010). *Russian J. Phys. Chem.*, *84*, 1158.
[10] Van der Spoel, D., Lindahl, E., Hess, B., van Buuren, A. R., Apol, E., Meulenhoff, P. J., Tieleman, D. P., Sijbers, A. L. T. M., Feenstra, K. A., van Drunen, R., & Berendsen, H. J. C. GROMACS User Manual version 3, 3.1//www.GROMACS.org.
[11] Agelmenev, M. E., Muldakhmetov, Z. M., Bratukhin, S. M., Pak, V. G., Polikarpov, V. V., & Yakovleva, O. A. (2008). *Mol. Cryst. Liq. Cryst.*, *494*, 339.
[12] Agelmenev, M. E., Muldakhmetov, Z. M., Bratukhin, S. M., Pak, V. G., Polikarpov, V. V., & Yakovleva, O. A. (2008). *Russian J. Phys. Chem. A*, *82*, 784.
[13] Oleg Kadkin, N., Eun, Ho Kim, Young, Joon Rha, So Yeon, Kim, Jigeon, Tae, & Moon-Gun, Choi. Electronic-Liquid Crystal Communications March 23, 2009, http://www.e-lc.org/docs/2009_03_16_23_16_14.
[14] de Gennes, P. G. (1974). *The Physics of Liquid Crystals*, Clarendon Press: Oxford.
[15] Agelmenev, M. E. (2002). *Kazakh Izv. NAN RK, Ser. Chem.*, *6*, 48.
[16] Muldakhmetov, Z. M., Agelmenev, M. E., & Sovetov, E. S. (1999). *Russian J. Phys. Chem.*, *73*, 1881.
[17] Agelmenev, M. E., Bazhikov, K. T., Muldakhmetov, Z. M., & Sizykh, M. Yu. (2002). *Russian J. Phys. Chem.*, *76*, 1713.