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GRZEGORZ W. BĄK

Institute of Physics, Lodz University of Technology, ul. Wólczańska 219, 90-924 Łódź, e-mail: grzegorz.bak@p.lodz.pl

COMPARISON OF SOME PROPERTIES AND MOLECULAR STRUCTURE OF MHPOBC AND CHLORINATED MHPOBC

Comparison of molecular structure of MHPOBC and chlorinated MHPOBC has been made and presented in the paper. The main difference in molecular structure of MHPOBC and chlorinated MHPOBC molecules consists in different properties of two chemical bonds between the benzene ring with substituted chlorine atom and neighbouring parts of molecule. For chlorinated version of MHPOBC the component of molecular dipole moment perpendicular to the long axis of molecule is substantially smaller than for MHPOBC molecules. As a result of chlorination core of MHPOBC molecules becomes more flexible. These differences of molecular structure lead to easily noticeable differences in macroscopic properties of MHPOBC and its chlorinated version.

Keywords: ferroelectric/antiferroelectric liquid crystals, molecular structure.

1. INTRODUCTION

Antiferroelectric liquid crystals (AFLC) are studied intensively during the last years both due to rich variety of interesting subphases and phase transitions detected in these materials and due to their possible practical applications. Till now numerous papers describing various properties of AFLC have been published (see for instance [1-9]). The attempt to derive liquid crystalline (LC) structure from electrostatic attractive forces (the van der Waals interaction) and the repulsive forces related to the excluded volume effect was presented to explain formation of the nematic phase [10,11]. Electrostatic interactions might be the deceive factor in case of nematic ferroelectrics (very few examples of such materials have been reported, see for instance Yen at.al. [12] and Koike et.al. [13]), but most antiferroelectric and ferroelectric LC phases cannot be described in this way. In order to form a ferroelectric structure it is necessary to have sufficiently low symmetry [9]. Bent-core liquid crystals are good example of systems possessing sufficiently low symmetry to form ferroelectric structures. Nevertheless, there is no doubt that both the electrostatic attractive forces and the repulsive forces influence formation of structural phases in LC materials. Deep discussion of appearance of LC ferroelectric and antiferroelectric phases has been presented in an important review paper [9]. However, though the knowledge of properties of AFLC materials has increased substantially during the last years, the understanding of relation between molecular structure of AFLC and their physical properties, in particular their phase sequence and temperatures of phase transitions is still not satisfactory.

4-(1-methyl-heptyloxy carbonyl) phenyl 4’-octyloxybiphenyl-4-carboxylate (MHPOBC) is the well-known standard AFLC material which has a rich sequence of helical phases. Its chlorinated analogue shows remarkable differences in phase sequence in comparison with the not chlorinated compound. The aim of this paper is to study the molecular structure of the two compounds, in particular charge distribution and stiffness of molecular core, to try to find the relation between their molecular structure and some macroscopic physical properties of these compounds.

2. COMPARISON OF PROPERTIES OF MHPOBC AND CHLORINATED MHPOBC

The following phase sequence for MHPOBC

$$\mathrm{SmA}^* - \mathrm{SmC}^*_\alpha - \mathrm{SmC}^*_\beta - \mathrm{SmC}^*_\gamma - \mathrm{SmC}^*_A$$

was suggested by Chandani et.al. [2]. The later experiments showed that the phase sequence of MHPOBC depends on the optical purity of material [5]. On decreasing of optical purity ordinary sinclinic SmC* phase appears from SmC$^*_\alpha$, SmC$^*_\beta$ and SmC$^*_\gamma$ subphases. Lagerwall and coworkers suggested the following phase sequence of (S)-MHPOBC obtained on heating [4]:

$\mathrm{Cr}(59^o\mathrm{C})\mathrm{SmC}^*_A(119.5^o\mathrm{C})\mathrm{SmC}^*_\gamma(120.5^o\mathrm{C})\mathrm{SmC}^*_\beta(121.9^o\mathrm{C})\mathrm{SmC}^*_\alpha(123.0^o\mathrm{C})\mathrm{SmA}^*$ (150.2)Iso

The material used was pure enough to show the smectic subphases characteristic of MHPOBC.

The first reports on chlorinated version of MHPOBC (see Fig.1) came from Furukawa et.al [14] and Sasaki et.al. [15]. The phase sequences and temperature ranges presented in the two papers were significantly different.

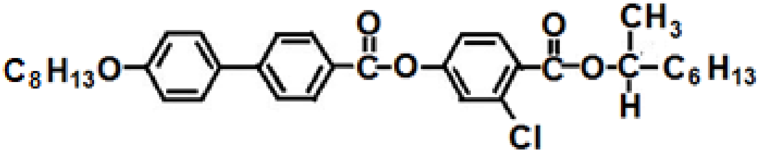

Fig. 1. Structure of chlorinated MHPOBC molecule

During the next years a few other papers concerning chlorinated MHPOBC have been published [8,16-19]. The phase sequence of chlorinated MHPOBC differs significantly from the phase sequence of MHPOBC. The following phase sequence on heating has been reported for chlorinated MHPOBC [16,17] and confirmed in other papers [18,19]:

Cr (26.4) SmC^*_{A} (97.0) SmC^*_{γ} (97.2)SmC^* (98.9) SmC^*_{α} (99.4) SmA^* (117.3) Iso

As it results from comparison of the phase sequences of MHPOBC and chlorinated MHPOBC the chlorinated version of MHPOBC shows various chiral SmC subphases, viz. SmC^*_{α}, SmC^* and SmC^*_{γ}, at substantially lower temperatures in comparison with MHPOBC (see Fig.2). The main advantage of chlorinated MHPOBC for potential application of this material in display devices consists in the presence of wide range room temperature antiferroelectric SmC^*_{A} phase. Not many compounds have been reported to show SmC^*_{A} phase in so broad temperature range comparatively close to room temperature [20].

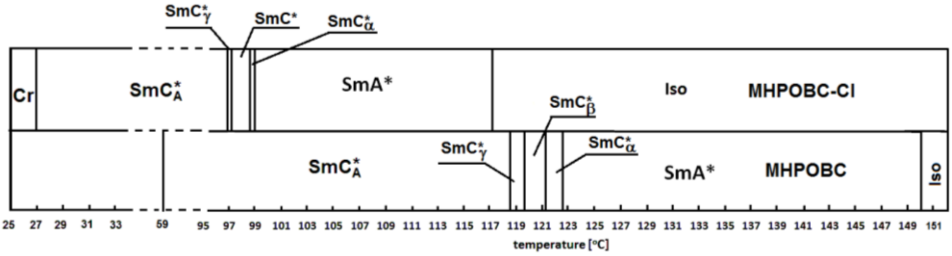

Fig. 2. Comparison of phase sequence of MHPOBC (lower part) and chlorinated MHPOBC (upper part)

3. MOLECULAR STRUCTURE OF MHPOBC AND CHLORINATED MHPOBC

If there exist no restrictions imposed on molecular motions in a physical system, different conformers of molecules forming the system co-exist in a dynamical equilibrium described by Boltzmann distribution:

$$\frac{N_i}{N} = \frac{exp\left(-\frac{E_i - E_{min}}{RT}\right)}{\sum_{k=1}^{N} exp\left(-\frac{E_k - E_{min}}{RT}\right)} \tag{1}$$

where N_i/N is the ratio of the i-th conformer to the total number of molecules at equilibrium, E_i is the energy of the i-th conformer, E_{min} is the minimum energy conformer, R is the molar gas constant and T is the temperature. In many cases the binding energy of a number of conformers is both minimal and exactly the same. First of all these conformers contribute to structure of molecular condensed matter on condition that molecules are quite free to move.

In case of liquid crystals, we have to do with free molecular motions in isotropic liquid. On cooling, the phase transitions probably consist of two steps:

- Freeze on translational motion. Molecules in frozen positions are not quite free to move due to intermolecular interactions with surrounding molecules and due to steric hindrance.
- Adjustment of molecular structure to frozen positions of surrounding molecules to find equilibrium point of minimal energy of a whole system. The adjustment depends on intra-molecular transitions between various conformers of molecules. The vibration frequency of intra-molecular vibrations is of the order of 10^{14} Hz, so the second step should be much faster than the first one on condition that the potential barriers between structure of different conformers is not high enough to slow down the transitions between various conformations of molecules.

In order to estimate the influence of chlorine atom on properties of chlorinated MHPOBC one should investigate the influence of the atom on formation of main conformers of chlorinated MHPOBC.

Molecules of MHPOBC are comparatively long and contain two COO polar groups. If we consider rotations of atoms around chemical bonds, some number of chemical bonds in MHPOBC molecule has more than one equilibrium position of the same binding energy of molecule. This means that there exist a number of conformers of the molecule of the same binding energy but different shape and may be of different dipole moment. In Fig. 3, the molecular structure of one of possible MHPOBC conformers is shown. Rotations around the six

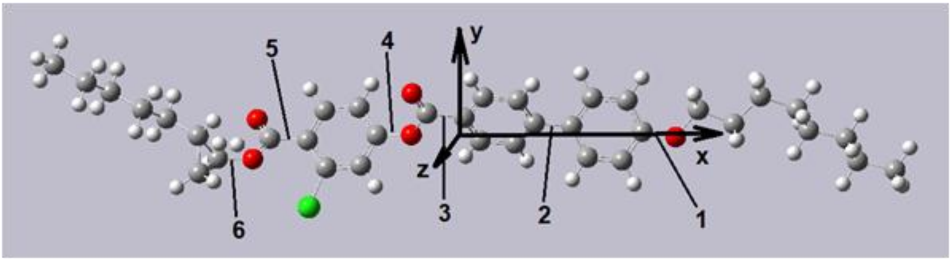

Fig. 3. Molecular structure of MHPOBC. Grey spheres: carbon atoms, red spheres: oxygen atoms, white spheres: hydrogen atoms. The bonds marked in the figure supposedly have particularly strong influence on dipole moment of the molecules. The green sphere is the chlorine atom in the chlorinated MHPOBC molecule.

bonds marked in the figure changes position of strongly electronegative oxygen atoms, so it may be supposed that these rotations influence the dipole moment of MHPOBC in particular. In the first step of the investigations the quantum calculations of these six bonds will be presented to find the equilibrium positions of atoms forming the bonds.

In order to find equilibrium states for the six chemical bonds chosen for the investigations, the molecular structure of the two molecules were optimized using Berny algorithm [21]. The calculations were carried out with the use of restricted Hartree-Fock model and the 6-31G(d,p) basis set. In order to verify the results a number of calculations were repeated using B3LYP model with the same 6-31G(d,p) set of functions. In the first step the molecules were optimized to obtain one of the possible conformers. In the next step scanning of rotations around the six bonds was carried out. The binding energy of molecule is a function of angle of rotation around the chosen bonds, the minima of binding energy define angles of equilibrium corresponding to a stable molecular conformer. Stability of a conformer depends on the potential barrier between neighbouring potential wells corresponding to other molecular conformers. It will be shown in the next part of the paper that the frequency of transitions between various conformational states of MHPOBC and chlorinated MHPOBC molecules is in a very broad range between picoseconds and approximately 10^{-2} s.

The calculations were carried out and the results were visualized using Gaussian 09 [22] software supported with GaussView 5.0 interface.

Figure 4 shows comparison of binding energies of MHPOBC and its chlorinated version as a function of rotations around bond 1. The bond is quite far from the chlorine atom, so as expected, the curves are very similar, two deep equilibrium states are detected at the dihedral angle 0° and 180°.

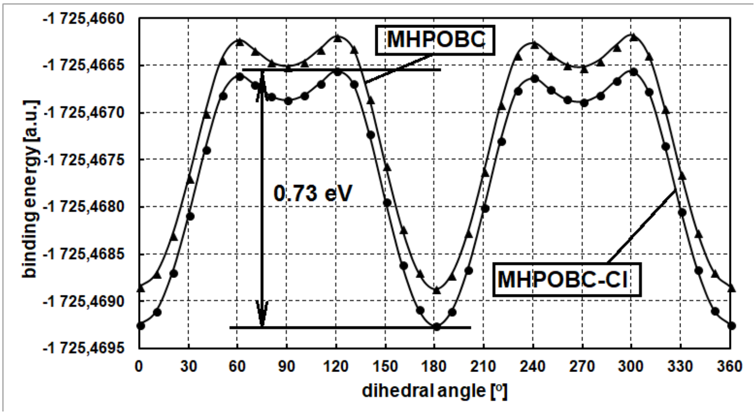

Fig.4.Comparison of the binding energy of MHPOBC and chlorinated MHPOBC as a function of rotation around bond 1. Two deep potential wells corresponding to equilibrium state at 0° and 180° are found. The data corresponding to chlorinated MHPOBC are shifted down for clarity. The barrier height between the two main equilibrium states of the bond equals 0.73 eV.

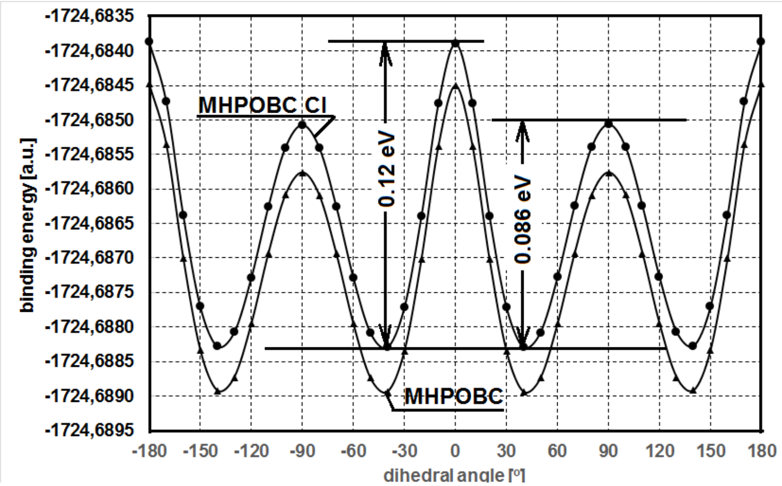

Fig. 5. Comparison of the binding energy of MHPOBC and chlorinated MHPOBC as a function of rotation around bond 2. Four deep potential wells corresponding to equilibrium states at approximately –140°, –40°, 40° and 140° are found. The data corresponding to chlorinated MHPOBC are shifted down for clarity. The barrier height between the four equilibrium states of the bond equals 0.12 eV and 0.086 eV.

Rotations around the bond between the two benzene rings (bond 2) change the relative directions of ester groups which gives the greatest contribution to the total dipole moment, so the rotations around this bond also influence the total molecular dipole moment. The two curves are very similar, the binding energy of bond 2 possesses 4 potential wells for both MHPOBC and its chlorinated counterpart with minima at approximately –140°, –40°, +40° and +140° (Fig.5, see also [23,24]). The barriers between the equilibrium states are comparatively low, their height is 0.12 eV and 0.086 eV. Rotations around the bond rather do not change bending of core because the two benzene rings lie on a straight line.

Rotations around bond 3 shows two equilibrium states at 0° and ±180° and no difference between MHPOBC and its chlorinated version has been found for this bond (see Fig.6).

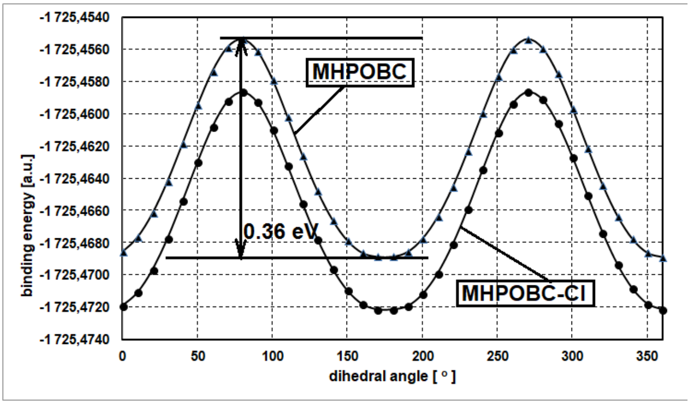

Fig. 6. Comparison of the binding energy of MHPOBC and chlorinated MHPOBC as a function of rotation around bond 3. Two deep potential wells corresponding to equilibrium states at 0° and 180° are found. The data corresponding to chlorinated MHPOBC are shifted down for clarity. The barrier height between the two main equilibrium states of the bond equals 0.36 eV.

Bonds 4 and 5 are close to the chlorine atom so it may be expected that the atom influences the properties of the bonds. And sure enough, for bond 4 a substantial difference is found between the two curves describing the relation between the binding energy and the dihedral angles describing the rotations around these bonds in MHPOBC and chlorinated MHPOBC (see Fig.7). Two main equilibrium positions corresponding to –120° and 120° are found for MHPOBC molecule, the binding energy for approximately ±70° does not create potential wells at these dihedral angles in principle. For chlorinated MHPOBC molecule only one main equilibrium position at approximately 60° is found. The change of binding energy as a function of the angle of rotation around bond 4

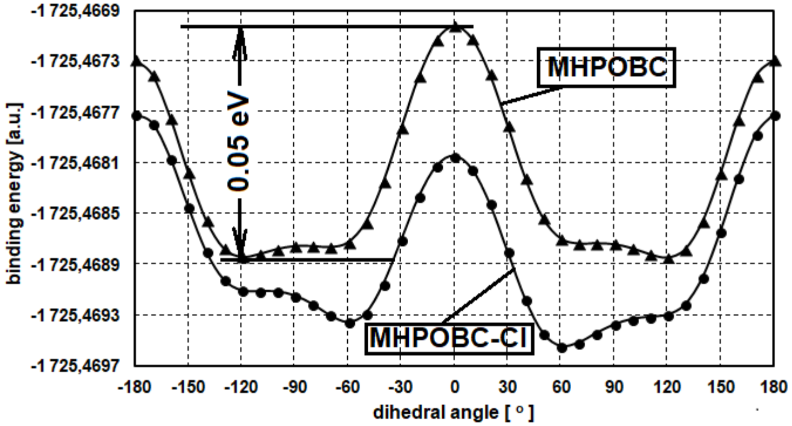

Fig.7. Comparison of binding energy of MHPOBC and chlorinated MHPOBC as a function of rotations around bond 4. Only one main minimum at about 60° is found in chlorinated MHPOBC while two main minima at ±120° for the not chlorinated version are found. The data corresponding to chlorinated MHPOBC are shifted down for clarity. The barrier between the equilibrium states in MHPOBC equals 0.05 eV, for chlorinated MHPOBC the barrier lowers to approximately 0.04 eV.

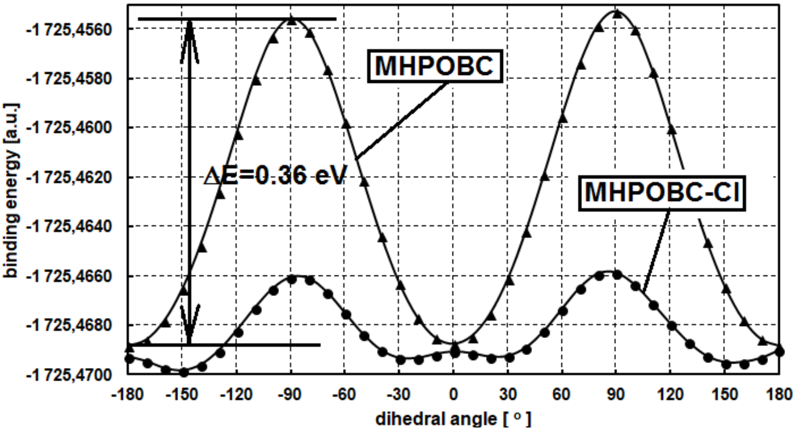

Fig. 8. Comparison of binding energy of MHPOBC and chlorinated MHPOBC as a function of rotations around bond 5. Two main equilibrium states at 0° and 180° are detected for MHPOBC, one main equilibrium state at –150° is detected for the chlorinated version, though the difference in the binding energy between the main state at –150° and the other one at +150° is rather small. The data corresponding to chlorinated MHPOBC are shifted down for clarity. The barrier between the equilibrium states in MHPOBC equals 0.36 eV, for chlorinated MHPOBC the barrier lowers to approximately 0.11 eV.

may result from additional polarisation of easily polarisable π-electrons of the benzene ring in the vicinity of strongly electronegative chlorine atom.

Similar effect is observed for bond 5. The curves describing the relation between the binding energy and the dihedral angles of rotations around bond 5 in MHPOBC and chlorinated MHPOBC also differs significantly (see Fig. 8). Instead of two main equilibrium states corresponding to 0^{o} and 180^{o} only one equilibrium state at -150^{o} remains, though the difference in the binding energy between the main position at -150^{o} and the other one at $+150^{o}$ is rather small. The minima of potential wells at approximately $\pm 30^{o}$ and at 150^{o} correspond to higher energies than that at -150^{o}, so they are more seldom occupied according to Boltzmann statistics though the difference in population of the four MHPOBC-Cl conformers is rather not substantial due to comparatively small difference in binding energies of the four conformers.

Comparison of properties of bond 6 in MHPOBC and chlorinated MHPOBC shows very weak influence of the chlorine atom on the bond (see Fig. 9). Two equilibrium states corresponding to -150^{o} and -90^{o} are found.

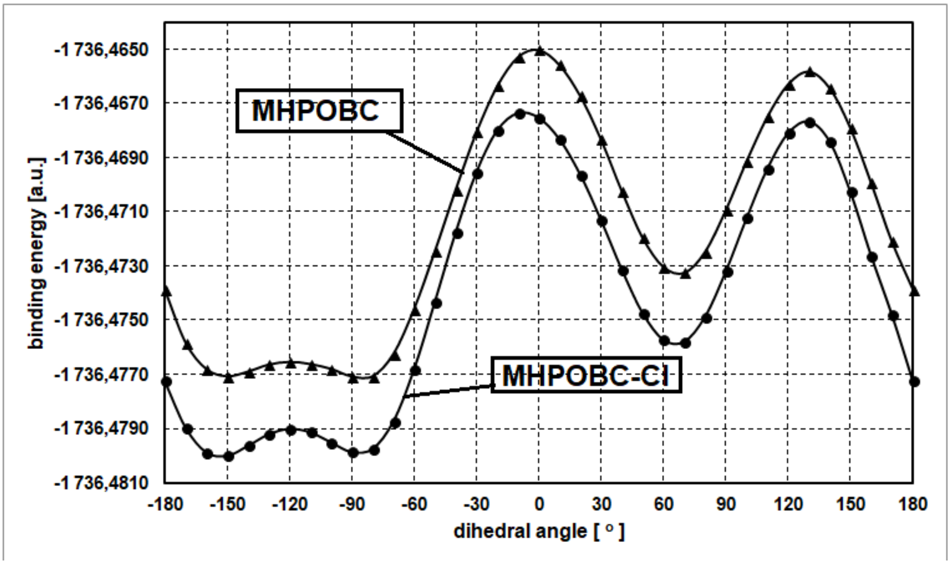

Fig. 9. Comparison of binding energy of MHPOBC and chlorinated MHPOBC as a function of rotations around bond 6. Two equilibrium positions corresponding to -150^{o} and -90^{o} are found. The data corresponding to chlorinated MHPOBC are shifted down for clarity.

For MHPOBC-Cl molecule the number of main equilibrium states for the 6 consecutive bonds is 2, 4, 2, 1, 1 and 2, so the number of different conformers corresponding to the states is equal to 2×4×2×1×1×2 = 32. Because both bond 4 and bond 5 for MHPOBC molecules possess not 1 but 2 main equilibrium positions, 4 additional conformers of MHPOBC molecule correspond to each of the 32 conformers of chlorinated MHPOBC molecule. In order to discuss the influence of chlorine atom on properties of MHPOBC molecule representative 4 out of 32 conformers of chlorinated MHPOBC have been chosen.

3.1. Charge distribution in molecules of MHPOBC and chlorinated MHPOBC

Table 1 shows comparison of charge distribution in MHPOBC and chlorinated MHPOBC for four representative conformers of chlorinated MHPOBC out of 32 its main conformers, marked with K1, K9, K14 and K25. The results and conclusions obtained for the four conformers may be regarded as typical for other conformers of the compound. Each of the four chosen conformers possesses four MHPOBC counterparts due to 2 additional equilibrium states of bonds 4 and 5 in MHPOBC molecule. The table shows the total value of molecular dipole moment of chlorinated MHPOBC and of the four corresponding conformers of MHPOBC and its *x*, *y* and *z* components. Additionally, the values of total dipole moments perpendicular to the long axis of molecule $D_{yz}=\sqrt{D_y^2+D_z^2}$ are also shown.

For chlorinated MHPOBC the D_{yz} components perpendicular to the long axis are comparatively small and equal to 1.75 D, 1.476 D, 1.502 D and 1.11 D for the four conformers chosen for the analysis. For MHPOBC corresponding conformers the situation is quite different. 14 out of 16 D_{yz} components of dipole moment for MHPOBC molecules are greater than 1.75 D, i.e. they are greater than the greatest value of D_{yz} component for chlorinated MHPOBC molecules. The only exceptions are D_{yz} components for K1.4 and K25.4 MHPOBC conformers. This means that as a result of chlorination the population of conformers possessing comparatively high value of dipole moment perpendicular to the long *x*-axis of molecule is substantially smaller, so the molecules possessing great dipole moment perpendicular to the long axis of molecule are not so easily available. It has been suggested that self-polarisation of liquid media is closely related to value of dipole moment perpendicular to the long axis of molecules [25], so this may be one of the reasons for so significant difference between phase sequence of MHPOBC and chlorinated MHPOBC.

Table 1

Comparison of charge distribution in MHPOBC and chlorinated MHPOBC[1]

MHPOBC-Cl		D_x [D]	D_y [D]	D_z=[D]	D [D] D_{yz} [D]
K1	b1=0;b2=140;b3=0;b6=-155; b5=-152;b4=62;	4.268	0.4793	-1.6827	4.6127 1.750
MHPOBC					
K1.1	b1=0;b2=140;b3=0;b6=-155; b5=0;b4=120;	3.519	-2.443	-0.202	4.289 2.451
K1.2	b1=0;b2=140;b3=0;b6=-155; b5=0;b4=-120;	3.53	-3.456	0.043	4.94 3,456
K1.3	b1=0;b2=140;b3=0;b6=-155; b5=180;b4=120;	3.514	1.723	2.222	4.501 2.812
K1.4	b1=0;b2=140;b3=0;b6=-155; b5=180;b4=-120;	3.492	-0.948	-0.908	3.734 1.313
MHPOBC-Cl					
K9	b1=180;b2=-140;b3=0; b6= -155; b5=-152;b4=62;	4.177	1.471	-0.12	4.431 1.476
MHPOBC					
K9.1	b1=180;b2=-140;b3=0; b6=-155; b5=0;b4=120;	3.246	4.635	0.497	5.680 4.660
K9.2	b1=180;b2=-140;b3=0; b6=-155; b5=0;b4=-120;	3.393	3.711	0.682	5.074 3.773
K9.3	b1=180;b2=-140;b3=0;b6= -155; b5=180;b4=120;	3.417	-0.684	1.708	3.881 1.840
K9.4	b1=180;b2=-140;b3=0;b6=-155; b5=180;b4=-120;	3.287	-3.322	-0.402	4.691 3.346
MHPOBC-Cl					
K14	b1=180;b2=40;b3=180;b6=-155; b5=-152;b4=62;	4.206	1.494	-0.155	4.466 1.502
MHPOBC					
K14.1	b1=180;b2=40;b3=180; b6=-155; b5=0;b4=120;	3.206	4.524	0.453	5.563 4.547
K14.2	b1=180;b2=40;b3=180; b6=-155; b5=0;b4=-120;	3.373	-3.495	-0.558	4.889 3.539
K14.3	b1=180;b2=40;b3=180;b6=-155; b5=180;b4=120;	3.413	-0.706	1.735	3.893 1.875
K14.4	b1=180;b2=40;b3=180;b6=-155; b5=180;b4=-120;	3.279	-3.358	-0.426	4.713 3.385

[1] *The origin of frame of reference is placed at the center of charge distribution on molecule, direction of the axes is along the main axes of tensor of charge distribution, x-axis is along the long axis of molecule. Depending on changing structure of molecule for consecutive conformers x-axis remains the long axis of molecule, the direction y- and z-axis can change. In consequence, only* D_{yz} *component, perpendicular to x-axis, should be regarded as characteristic for a specific conformer, because y- and z- components may change with changing direction of y- and z-axis.*

MHPOBC-Cl					
K25	b1=180;b2=-140;b3=0;b6=-85; b5=-152;b4=62;	4.334	1.017	0.445	4.474 1.110
MHPOBC					
K25.1	b1=180;b2=-140;b3=0;b6=-85; b5=0;b4=120;	3.547	2.517	0.156	4.353 2.522
K25.2	b1=180;b2=-140;b3=0;b6=-85; b5=0;b4=-120;	3.585	3.3	0.732	4.927 3.380
K25.3	b1=180;b2=-140;b3=0;b6=-85; b5=180;b4=120;	3.6	1.815	1.992	4.497 2.695
K25.4	b1=180;b2=-140;b3=0;b6=-85; b5=180;b4=-120;	3.574	-0.772	-1.047	3.804 1.301

3.2. Stiffness of molecular core of MHPOBC and chlorinated MHPOBC molecules

As suggested above, the phase transition in LC consists of 2 steps. After freeze on translational motion of molecules the next step consists in adjustment of shape of molecules to the frozen structure. The relaxation time τ of the adjustment is given by:

$$\tau^{-1} = {}_{vib}e^{\frac{-\Delta E}{kT}} \tag{2}$$

where *ΔE* is the barrier height, ν_{vib} is the frequency of attempts to overcome the barrier, *k* is the Boltzmann constant and T is the temperature. The barrier height between various main equilibrium positions of the considered bonds changes in the range between 0.76 eV for bond 1, 0.36 eV for bond 5 and 0.04 eV for bond 4. Assuming $\nu_{vib} = 10^{14}$ Hz (frequency of intramolecular vibrations) we get in the vicinity of room temperature the relaxation times in a very wide range between picoseconds and approximately 10^{-2} s.

Though existence of bent-core molecular conformers supports formation of various LC ferroelectric structures, it is not enough. According to the suggested above two-step model of phase transitions the crucial factor is whether bent-core molecular conformers form a LC structure of binding energy low enough to stabilize the structure. To some extent this depends on easiness of transitions between various conformational states of molecules to stabilize the whole structure.

The difference between population of MHPOBC and chlorinated MHPOBC molecules consists in the differences in equilibrium states of bonds 4 and 5 (see Fig. 3). In case of bond 5 for MHPOBC molecule two deep equilibrium states of the bond separated with the barrier 0.36 eV high are replaced by four comparatively shallow equilibrium states of slightly different binding energies in chlorinated MHPOBC molecule. The barrier height between the states is much lower and equal to about 0.11 eV. According to Eq. (1) rotations around bond 5 in chlorinated MHPOBC becomes faster by approximately 5 orders of magnitude at the vicinity of room temperature. This makes rotations of these endings of chlorinated MHPOBC molecule much easier. As a result, MHPOBC-Cl molecules can adjust to the frozen structure much easier.

In case of bond 4 two main equilibrium states of the bond at $\pm 120^{o}$ in MHPOBC molecule are replaced by only one main equilibrium state at $+60^{o}$ in molecule of chlorinated MHPOBC. The barrier height between neighbouring equilibrium states decreases as a result of chlorination from 0.05 eV for MHPOBC molecules down to 0.04 eV for the chlorinated version of MHPOBC. These barrier heights are comparable with the thermal energies in the temperature range used. The lower barrier between potential wells in chlorinated MHPOBC molecule means that transitions between neighbouring stable states becomes nearly twice faster than in its MHPOBC counterpart. Having in mind that bond 4 influences shape and stiffness of molecular core we can conclude that cores of chlorinated MHPOBC molecules are more flexible in comparison to their MHPOBC counterparts.

It results from the data shown in Table 1 that the component of dipole moment perpendicular to the long molecular axis is in general smaller for the chlorinated MHPOBC molecules. However, the experimental value of $\varepsilon'_{\perp}$ for Cl-MHPOBC proves to be higher for the chlorinated version (see [16] for instance). The value of dielectric permittivity reflects value of charge induced as a result of external electric field. In case of polar materials the value of induced charge depends not only on value of dipole moment, but also on mobility of charge to adjust to external electric field. This suggests that flexibility of the chlorinated molecules influences the induction of polarisation charge first of all.

4. SUMMARY

The following main conclusions can be put forward as a result of the above calculations and discussion:

1. Substitution of the hydrogen atom by chlorine atom in MHPOBC molecule (see Fig. 3) leads to substantial decrease in value of the component of dipole moment perpendicular to the long axis of molecule. Values of dipole moment perpendicular to the long axis of molecules D_{yz} in chlorinated MHPOBC conformers are much smaller than in its MHPOBC counterparts.
2. The difference between population of MHPOBC and chlorinated MHPOBC molecules consists in the differences in equilibrium states of two bonds

marked with 4 and 5 (Fig.3). In case of bond 4 two main equilibrium states of bond 4 at ±120° in MHPOBC molecule are replaced by only one main equilibrium state at +60° in molecule of chlorinated MHPOBC. Due to lower energy barriers between available equilibrium states core of chlorinated MHPOBC molecules becomes more flexible.

3. In case of bond 5 in MHPOBC molecule two deep equilibrium positions of the bond separated with the barrier 0.36 eV high are replaced by four much shallower equilibrium positions of slightly different binding energies in chlorinated MHPOBC molecule. As a result, rotations of these endings of chlorinated MHPOBC molecules become much easier.
4. Two factors are considered to be crucial for formation of polar structures in liquid crystalline materials, i.e. sufficiently low symmetry of molecules and electrostatic interaction between molecules. However, considering symmetry of molecules their stiffness should also be taken into account. When translational motion becomes frozen, adjustment of molecules into structure depends on easiness of transitions between available molecular conformations. It seems that so substantial differences in the phase sequences of MHPOBC and chlorinated MHPOBC may result both from change of charge distribution on molecules and from substantial difference in stiffness of molecular core of the two molecules.
5. The next and not easy step in investigations of relation between molecular and macroscopic structure of molecular condensed matter is to find the way to calculate a macroscopic structure for a given molecular structure of compound forming the matter.

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PORÓWNANIE NIEKTÓRYCH WŁAŚCIWOŚCI I STRUKTURY MOLEKULARNEJ MHPOBC I CHLOROWANEGO MHPOBC

Streszczenie

Porównano strukturę molekuły i niektóre właściwości fizyczne MHPOBC i MHPOBC-Cl Podstawowa różnica struktury molekuły polega na różnicy właściwości dwu wiązań chemicznych pomiędzy pierścieniem benzenowym zawierającym atom chloru a sąsiednimi fragmentami molekuły. Dla chlorowanej wersji MHPOBC obliczona składowa momentu dipolowego prostopadła do

długiej osi molekuły jest istotnie mniejsza niż w przypadku molekuły MHPOBC. W wyniku zmiany właściwości niektórych wiązań molekuła MHPOBC-Cl staje się mniej sztywna. Konsekwencją tych różnic właściwości molekuł są istotne różnice właściwości fizycznych obydwu substancji.