Influence of Molecule Core Change on its Properties

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Influence of Molecule Core Change on its Properties

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Three quantities characterising a liquid crystal molecules were voted to
study their physical properties. The $(\alpha_\parallel - \alpha_\perp)$ of liquid crystals
investigated is almost constant at all range of mesophase, but they have
a different values for each molecule of liquid crystals. It prove the
change of molecule core of liquid crystal influence on their
polarizability tensor components. The subject of this work was a three
liquid crystal of CB 7, PCH 7 and CCH 7. Molecule core change has
clearly influenced on the values of $(\alpha_\parallel - \alpha_\perp)$. Components of
polarizability tensor of molecule $\alpha_\parallel$, $\alpha_\perp$ were calculated too.

Keywords: liquid crystals; polarizability tensor; molecule properties.

INTRODUCTION

Liquid crystals belong to the chemical compounds, which have found great

number of applications in technique and in everyday life. They have

properties of both states of solid and liquid one. Main features of liquid

crystals are a anisotropy of dielectric permittivity, refractive indices and

viscosity. If we want to investigate the liquid crystal properties we must have

a information about liquid crystal molecules. As we know the liquid crystal

molecules change their conformations with the change of temperature[1-3]

because the molecular interaction is changed in this case. Studies of molecular structure and properties belong to the difficult problems. A few methods exist in the literature[2-13], which are useful in calculation of α_s, $\alpha_{\parallel}$, $\alpha_{\perp}$ and $(\alpha_{\parallel}-\alpha_{\perp})$ belonged to the liquid crystal molecules. If we want to study of physical properties of molecule, three quantities may be use for this aim.

TABLE I. Order parameter S, anisotropy of polarizability tensor components of $(\alpha_{\parallel}-\alpha_{\perp})$ and polarizability tensor components of $\alpha_{\parallel}$ and $\alpha_{\perp}$ of CB 7.

ΔT	$(n_e+n_o)/d$	$S=k_A\Delta n$	$(\alpha_{\parallel}-\alpha_{\perp})10^{23}cm^3$	$\alpha_{\parallel}10^{23}cm^3$	$\alpha_{\perp}10^{23}cm^3$
13	3.219	0.700	38.329	94.898	56.569
11.5	3.219	0.685	38.339	94.791	56.455
10	3.220	0.673	38.350	94.734	56.384
8.5	3.222	0.661	38.372	94.696	56.325
7	3.227	0.0642	38.426	94.715	56.289
6	3.223	0.619	38.380	94.588	56.208
5	3.224	0.607	38.387	94.513	56.126
3	3.225	0.568	38.404	94.458	56.054
1	3.223	0.514	38.384	94.195	55.810
0.5	3.225	0.479	38.404	94.386	55.982
-0.4	3.197	-	38.068	94.366	56.298
-3	3.202	-	38.116	94.275	56.158
-6	3.208	-	38.201	94.384	56.183
-11	3.216	-	38.288	94.288	55.999

One of them is the moment of inertia of molecule, but this quantity is very hard to a investigation. The second one is the trace of polarizability tensor of molecule. The tensor trace values do not depend on the coordinates systems and it can be a measure of change of the molecule conformation[4-10]. The

third quantity, which characterizes the liquid crystal molecule, is a polarizability tensor components of molecule of $\alpha_\parallel$, $\alpha_\perp$ and $(\alpha_\parallel - \alpha_\perp)$[11,12]. The $(\alpha_\parallel - \alpha_\perp)$ is especially important quantity, because it has evident a constant values at the all temperature range of mesophase and isotropic liquid state. The $(\alpha_\parallel - \alpha_\perp)$ may be used to a study of a influence of a core change of molecule on its properties. There are a three liquid crystals as CB 7, PCH 7, CCH 7, which molecules differ themselves by the change of one benzene ring on the hexil one. The molecule of CB 7 have a two benzene rings in its core but PCH 7 only one. On the contrary molecule of CCH 7 have only two hexil rings. In this work we want to study of $(\alpha_\parallel - \alpha_\perp)$, $\alpha_\parallel$ and $\alpha_\perp$ of mentioned above liquid crystal molecule, in order to obtain a information, how the core change of molecule influence on its physical properties and additionally to obtain the temperature dependence of polarizability tensor components of $\alpha_\parallel$ and $\alpha_\perp$. We want to notice that many scientists tried up to now to study of $(\alpha_\parallel - \alpha_\perp)$ by the use of Kerr effect without the good results.

THEORETICAL PART

In our previous work[13,14] it was proved that the trace of polarizability tensor of α_s of liquid crystal sample is equal to the α_s of liquid crystal molecule. It gives the equation:.

$$\alpha_s = (\alpha_\parallel + 2\,\alpha_\perp) = (\alpha_1 + 2\alpha_2). \tag{1}$$

If we want to calculate $\alpha_\parallel$ and $\alpha_\perp$ we ought to have an additional equation with these quantities. That equation may be the expression for a order parameter S of liquid crystal[15,16]. It has a mathematical form:.

$$(\alpha_1 - \alpha_2)/(\alpha_\parallel - \alpha_\perp) = S = k_A \Delta n \tag{2}$$

Solving equations (1) and (2) you can obtain the new expressions for $\alpha_\parallel$ and $\alpha_\perp$, if the value of k_A is known. In this case we find:.

$$\alpha_\parallel = (M/N)[(n^2-1)/d + 2(n_e + n_o)/3k_A d].$$

$$\alpha_\perp = (M/N)[(n^2-1)/d - (n_e+n_o)/3k_Ad].\tag{3}$$

Where M -molecular weight, N -Avogadro number, d - density of liquid crystal $n^2=(n_e^2+2n_o^2)/3$. From equation (3) we can receive a new one for a $(\alpha_\parallel-\alpha_\perp)$. On the end we receive the relation:.

$$(\alpha_\parallel-\alpha_\perp)=(M/N)(n_e+n_o)/k_Ad\tag{4}$$

TABLE II. Order parameter S, anisotropy of polarizability tensor components of $(\alpha_\parallel-\alpha_\perp)$ and polarizability tensor components of $\alpha_\parallel$ and $\alpha_\perp$ of PCH 7.

ΔT	$(n_e+n_o)/d$	$S=k_A\Delta n$	$(\alpha_\parallel-\alpha_\perp)10^{23}cm^3$	$\alpha_\parallel 10^{23}cm^3$	$\alpha_\perp 10^{23}cm^3$
26.5	3.232	0.7	23.462	80.581	57.119
23.5	3.236	0.68	23.488	80.545	57.058
20.5	3.240	0.67	23.519	80.482	56.962
17.5	3.244	0.64	23.548	80.423	56.875
14.5	3.249	0.62	23.582	80.368	56.786
11.5	3.255	0.60	23.629	80.434	56.805
8.5	3.259	0.564	23.656	80.336	56.681
5.5	3.264	0.518	23.691	80.344	56.653
3.5	3.267	0.49	23.713	80.294	56.581
1.5	3.267	0.43	23.716	80.137	56.419
0.5	3.314	0.40	24.053	80.349	56.296
-0.5	3.263	-	23.686	80.424	56.739
-2.5	3.267	-	23.715	80.416	56.701
-5.5	3.272	-	23.751	80.309	57.551
-10.5	3.281	-	23.815	80.313	56.488

k_A is a constant coefficient of proportionality between the order parameter S and refractive anisotropy of Δn. From equation (4) we can verify the temperature dependence of $(\alpha_\parallel-\alpha_\perp)$, if we have the values of n_e, n_o and density

d. In the experimental part we give in responsible tables the values of relation $(n_e+n_o)/d$ for three mentioned above liquid crystals. This quantity does not almost depend on temperature. It proves that $(\alpha_{\parallel}-\alpha_{\perp})$ is almost constant too. In order to check it we decided to calculate the $(\alpha_{\parallel}-\alpha_{\perp})$ for our liquid crystals. If we want to do it we must got the values of k_A for these liquid crystals. In the next part of our article we describe how we found it.

EXPERIMENTAL PART

In order to calculate the interested us quantities for CB 7, PCH 7, and CCH 7 we took the experimental data of refractive indices and density from our recent work[2]. In the Tables I , II, III there are collected all these values of new quantities, which we calculated in this work. As we written later k_A coefficient is very important for our calculation of $(\alpha_{\parallel}-\alpha_{\perp})$., but we do not know it for our liquid crystals. Up to now we know only two liquid crystals for which the k_A coefficient was experimentally definite. It was for cholesteryl nonanoate and decanoate[11,12]. Order parameter S of all liquid crystals is contained between 0.3 and 0.7. In this work we assume that the S value will be equal 0.7 for a maximal refractive anisotropy. Then having S and (n_e-n_o) we have calculated the k_A for our liquid crystals. The values obtained for k_A are: for CB 7 $k_A=3.867$, for PCH 7 $k_A= 6.481$ and for CCH 7 $k_A= 15.217$. We see the values of k_A are very different for our liquid crystals. Having now a k_A we can calculate the quantities us interested for same points of temperature of mesophase and isotropic liquid state. The results of these calculations are collected in the Table I, II, III, In these Tables we see that the $\alpha_{\parallel}-\alpha_{\perp}$ is almost constant for each liquid crystals, but its values are different. On the contrary the new expression $(n_e+n_o)/d$ is almost identical for all liquid crystals. The $\alpha_{\parallel}$ and $\alpha_{\perp}$ are depended on the temperature. They values are different for each liquid crystal investigated. In order to see better the difference or agreement of these data we constructed a Table IV from

data belonged to the lowest temperature of mesophase of our liquid crystals. In the Table IV we see the core change of liquid crystal molecules influence strongly on the $\alpha_{\|}-\alpha_{\perp}$, $\alpha_{\|}$, k_A, Δn and d values. The new expression of $(n_e+n_o)/d$ is almost constant and have the same values for liquid crystal

TABLE. III Order parameter S, anisotropy of polarizability tensor components of $(\alpha_{\|}-\alpha_{\perp})$ and polarizability tensor components of $\alpha_{\|}$ and $\alpha_{\perp}$ of CCH 7

ΔT	$(n_e+n_o)/d$	$S=k_A\Delta n$	$(\alpha_{\|}-\alpha_{\perp})10^{23}cm^3$	$\alpha_{\|}10^{23}cm^3$	$\alpha_{\perp}10^{23}cm^3$
13	3.312	0.7	10.457	69.660	59.203
10.4	3.315	0.65	10.468	69.516	59.048
8.4	3.318	0.59	10.476	69.457	58.981
6.3	3.320	0.563	10.484	69.312	58.828
4.3	3.322	0.487	10.489	69.179	58.690
2.4	3.327	0.457	10.505	69.223	58.718
1.5	3.330	0.411	10.514	69.179	58.666
0.5	3.330	0.350	10.514	69.050	58.536
-0.5	3.338	-	10.540	69.499	58.879
-2.5	3.343	-	10.556	69.425	58.848
-5.5	3.349	-	10.576	69.421	58.845
-10.5	3.357	-	10.599	69.218	58.619

investigated. In our opinion these different reactions on the core change of liquid crystal molecule are correct, because collected quantities in Table IV are combined with the different phenomenon. The $\alpha_{\|}-\alpha_{\perp}$, $\alpha_{\|}$ and $\alpha_{\perp}$ describe the answer of molecule on the electric field, which create the dipole moment of molecule. The change of molecule core of our liquid crystals causes a change of molecule structure and polarizability tensor components of $\alpha_{\|}$ and $\alpha_{\perp}$. The refractive indices and density are interrelated for a structure of

molecule. At Tab. IV we see same quantities values decrease with the change

of benzene ring on the hexil one. To these quantities belong the $(\alpha_{\parallel}-\alpha_{\perp})$, $\alpha_{\parallel}$,

Δn and density d. The quantities $(n_e+n_o)/d$, k_A, and $\alpha_{\perp}$ are slightly increasing

with the number of hexil rings. We see that $(n_e+n_o)/d$, for CB 7 and CCH 7

are almost similar, when the values of k_A for these liquid crystals are changed

TABLE IV. Collected quantities $\alpha_{\parallel}-\alpha_{\perp}$, $\alpha_{\parallel}$ and so on of CB 7, PCH 7 and
CCH 7 for lowest temperature of mesophase.

	$\alpha_{\parallel}-\alpha_{\perp}$	$\alpha_{\parallel}$	$\alpha_{\perp}$	k_A	$(n_e+n_o)/d$	Δn	d g/cm^3
CB 7	38.329	94.898	56.569	3.867	3.219	0.181	1.002
PCH 7	23.462	80.581	57.119	6.481	3.232	0.108	0.952
CCH 7	10.457	69.660	59.203	15.217	3.315	0.046	0.893

about 11.35. On the end we can notice that all investigated quantities are

changed, when the number of hexil rings increase in core of molecule. We

can say that $(\alpha_{\parallel}-\alpha_{\perp})$ is very important quantity, because it is independent of

temperature and therefore it may be a visit cart of molecule.

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