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POLARISABILITY TENSOR OF CB 5 MOLECULE AND LIGHT WAVELENGTH

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The influence of the wavelength of light on the values of polarisability tensor components $\alpha_{\parallel}$, $\alpha_{\perp}$, polarisability anisotropy $(\alpha_{\parallel} - \alpha_{\perp})$ and the order parameter S of liquid crystal molecules was verified. The refractive indices are functions of temperature and light wavelength. The values $\alpha_{\parallel}$ and $\alpha_{\perp}$ of a liquid crystal molecule can be calculated from refractive indices, density, and coefficient in the Valentova equation. Here, it was found that there is a relation between the wavelengths of the light and values of $(\alpha_{\parallel} - \alpha_{\perp})$ and $\alpha_{\parallel}$, $\alpha_{\perp}$ of CB 5 molecule. The values of the order parameter S obtained for CB 5 liquid crystal are identical for all wavelengths of light.

Keywords: liquid crystals; order parameter; polarisability tensor; polarisability anisotropy of molecule; wavelength of light

1. INTRODUCTION

Birefringence properties of liquid crystals are characterised by two polarisability tensors. The first is the polarisability tensor of a liquid crystal sample, described by the components α_1 and α_2. These components can be calculated from the refractive indices by using the equations proposed recently [1–4], or by using Lorenz-Lorentz', Vuks' and Neugebauer's equations [5]. The second polarisability tensor, with components $\alpha_{\parallel}$ and $\alpha_{\perp}$, is connected with the liquid crystal molecule. In 1961, Saupe and Maier used $\alpha_{\parallel}$ and $\alpha_{\perp}$ in their theory of orientational order of liquid crystal molecules

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[6]. As a result of the theory, the equations combining α_1 and α_2 with $\alpha_\parallel$, $\alpha_\perp$, and order parameter S of the molecules are:

$$\alpha_1 = \alpha_s/3 + (2/3)(\alpha_\parallel - \alpha_\perp)\,S$$

and

$$\alpha_2 = \alpha_s/3 - (1/3)(\alpha_\parallel - \alpha_\perp)\,S,$$

where α_s is the trace of polarisability tensor of a liquid crystal molecule. It is well known in the literature [1–4,7–8] that the refractive indices are functions of temperature and wavelength of light. Up to now the relation between polarisability tensor components $\alpha_\parallel$, $\alpha_\perp$, the polarisability anisotropy $(\alpha_\parallel - \alpha_\perp)$, and the light wavelengths has not been considered in our investigations. In this article, the influence of the wavelength of light on the values of polarisability tensor components $\alpha_\parallel$, $\alpha_\perp$, polarisability anisotropy $(\alpha_\parallel - \alpha_\perp)$, and the order parameter S of liquid crystal molecules is verified.

2. STUDIED COMPOUND AND METHODS USED

The subject of our investigation is the liquid crystalline material p-cyano-p-pentylbiphenyl abbreviated as CB 5. The molecules of this liquid crystal are composed of two benzene rings, CN group and alkyl chain. The benzene rings and CN group are the rigid part of the molecule but the benzene rings can turn around each other due to the existence of a single chemical bond between them. The alkyl chain can change its conformation by the change of the sample temperature. Previous studies of the above mentioned liquid crystal [4,7] don't take into account the dependence of polarisability tensor components on the wavelength of the light. The experimental data for our calculations, namely the refractive indices and density of a CB 5 molecule were taken from Ref. 9 for three wavelengths of the light: 5461 Å, 5893 Å, and 6328 Å. The respective data are collected in Tables 1, 2 and 3. Details of the computations of polarisability anisotropy $(\alpha_\parallel - \alpha_\perp)$, polarisability tensor components $\alpha_\parallel$ and $\alpha_\perp$, and order parameter S of liquid crystal molecules from the refractive indices and density data is described in Refs. 1–4. Basis equations for the calculations are:

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

TABLE 1 Refractive Indices n_e and n_o, Density of the Liquid Crystal d, Polarisability Anisotropy $(\alpha_\parallel - \alpha_\perp)10^{-23}\,cm^3$, Polarisability Tensor Component $\alpha_\parallel 10^{-23}\,cm^3$, and Order Parameter S of CB 5 for the Wavelength of the Light 5461 Å ($k_A = 3.0992$)

ΔT	$d, g/cm^3$	n_o	n_e	$(\alpha_\parallel - \alpha_\perp)10^{-23}\,cm^3$	$\alpha_\parallel 10^{-23}\,cm^3$	S
14.6	1.0266	1.536	1.739	42.62	92.17	0.629
14.4	1.0264	1.536	1.737	42.60	92.08	0.623
13.1	1.0252	1.537	1.734	42.63	92.11	0.611
12.2	1.0244	1.538	1.733	42.66	92.22	0.604
10.7	1.0236	1.539	1.727	42.63	92.05	0.583
10.3	1.0230	1.539	1.727	42.65	92.11	0.583
8.2	1.0206	1.540	1.721	42.69	92.08	0.561
7.6	1.0202	1.541	1.718	42.68	92.05	0.549
6.0	1.0184	1.542	1.714	42.71	92.08	0.533
5.4	1.0179	1.542	1.712	42.71	92.02	0.527
3.5	1.0160	1.544	1.703	42.70	91.88	0.493
2.8	1.0154	1.546	1.699	42.70	91.90	0.474
1.4	1.0315	1.550	1.689	42.70	91.89	0.431
0.1	1.0119	1.557	1.670	42.61	91.65	0.350

where M is the molecular weight of the molecule, N is the Avogadro number, d is the density of the liquid crystal, n_e and n_o are the refractive indices of extraordinary and ordinary light, respectively,

TABLE 2 Refractive Indices n_e and n_o, Density of the Liquid Crystal d, Polarisability Anisotropy $(\alpha_\parallel - \alpha_\perp)10^{-23}\,cm^3$, Polarisability Tensor Component $\alpha_\parallel 10^{-23}\,cm^3$, and Order Parameter S of CB 5 for the Wavelength of the Light 5893 Å ($k_A = 3.2098$)

ΔT	$d, g/cm^3$	n_o	n_e	$(\alpha_\parallel - \alpha_\perp)10^{-23}\,cm^3$	$\alpha_\parallel 10^{-23}\,cm^3$	S
14.6	1.0266	1.532	1.727	40.95	90.17	0.626
14.4	1.0264	1.532	1.726	40.95	90.13	0.623
13.1	1.0252	1.532	1.723	40.96	90.08	0.613
12.2	1.0244	1.533	1.722	40.99	90.18	0.607
10.7	1.0236	1.533	1.716	40.94	89.92	0.587
10.3	1.0230	1.534	1.716	40.98	90.07	0.584
8.2	1.0206	1.535	1.711	41.03	90.10	0.565
7.6	1.0202	1.536	1.707	41.01	90.01	0.549
6.0	1.0184	1.536	1.703	41.02	89.95	0.536
5.4	1.0179	1.537	1.701	41.03	89.97	0.526
3.5	1.0160	1.539	1.693	41.03	89.89	0.494
2.8	1.0154	1.541	1.685	40.98	89.69	0.462
1.4	1.0315	1.544	1.679	41.02	89.81	0.433
0.1	1.0119	1.551	1.662	40.96	89.68	0.356

TABLE 3 Refractive Indices n_e and n_o, Density d, Polarisability Anisotropy $(\alpha_\parallel - \alpha_\perp)10^{-23}\,cm^3$, Polarisability Tensor Component $\alpha_\parallel 10^{-23}\,cm^3$, and Order Parameter S of CB 5 for the Wavelength of the Light 6328 Å ($k_A = 3.2648$)

ΔT	$d, g/cm^3$	n_o	n_e	$(\alpha_\parallel - \alpha_\perp)10^{-23}\,cm^3$	$\alpha_\parallel 10^{-23}\,cm^3$	S
14.6	1.0266	1.528	1.719	40.11	88.91	0.624
14.4	1.0264	1.528	1.717	40.09	88.82	0.617
13.1	1.0252	1.528	1.714	40.10	88.76	0.607
12.2	1.0244	1.528	1.713	40.12	88.78	0.604
10.7	1.0236	1.530	1.708	40.12	88.75	0.581
10.3	1.0230	1.530	1.708	40.14	88.81	0.581
8.2	1.0206	1.531	1.702	40.17	88.78	0.558
7.6	1.0202	1.531	1.698	40.14	88.60	0.545
6	1.0184	1.532	1.695	40.18	88.68	0.532
5.4	1.0179	1.533	1.693	40.19	88.71	0.522
3.5	1.0160	1.535	1.685	40.19	88.63	0.490
2.8	1.0154	1.537	1.68	40.18	88.59	0.467
1.4	1.0315	1.540	1.672	40.19	88.60	0.431

$n^2 = (n_e^2 + 2n_o^2)/3$, and k_A is the coefficient in the Valentova equation [10,11].

The quantities $\alpha_\parallel$, $\alpha_\perp$ and $(\alpha_\parallel - \alpha_\perp)$ for the liquid crystal CB 5 were calculated from the values of its refractive indices, the density d, and the coefficient k_A. The accuracy in the measurements of Δn_e and Δn_o is 10^{-3} while that of Δd is $10^{-3}\,g/cm^3$. The relative error in the estimation of the polarisability anisotropy $(\alpha_\parallel - \alpha_\perp)$ calculated from these data is 0.002. Taking a typical value of $(\alpha_\parallel - \alpha_\perp)$ equal to 40. $10^{-23}\,cm^3$, one obtains $\Delta(\alpha_\parallel - \alpha_\perp) = 0.08.10^{-23}\,cm^3$.

3. DISCUSSION

Values of polarisability anisotropy $(\alpha_\parallel - \alpha_\perp)$ and polarisability tensor component $\alpha_\parallel$ for three wavelengths of light are listed in Tables 1, 2 and 3, respectively. The calculated values of $(\alpha_\parallel - \alpha_\perp)$ and $\alpha_\parallel$ versus the reduced temperature (ΔT) are presented additionally on Figure 1 and Figure 2, respectively. The reduced temperature can be expressed as $\Delta T = T_o - T$, where the T_o is the temperature of the phase transition to the isotropic phase and T is the temperature of the measurement for the mesophase.

The examination of Figure 1 reveals that the value of $(\alpha_\parallel - \alpha_\perp)$ is practically constant in the entire temperature range of measurements. However, there is a great influence of the wavelength of light on the

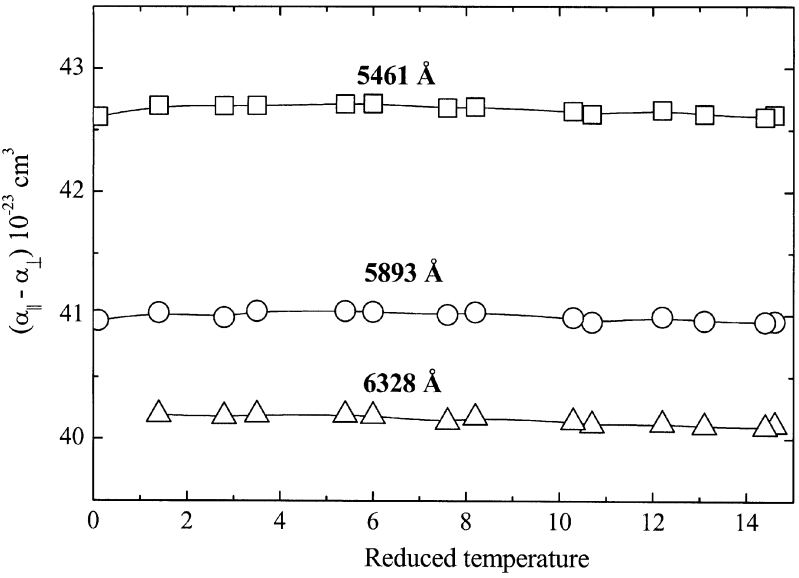

FIGURE 1 Polarisability anisotrophy $(\alpha_{\parallel} - \alpha_{\perp})10^{-23}\,\mathrm{cm}^3$ of CB 5 molecule as a function of the reduced temperature and the wavelength of the light.

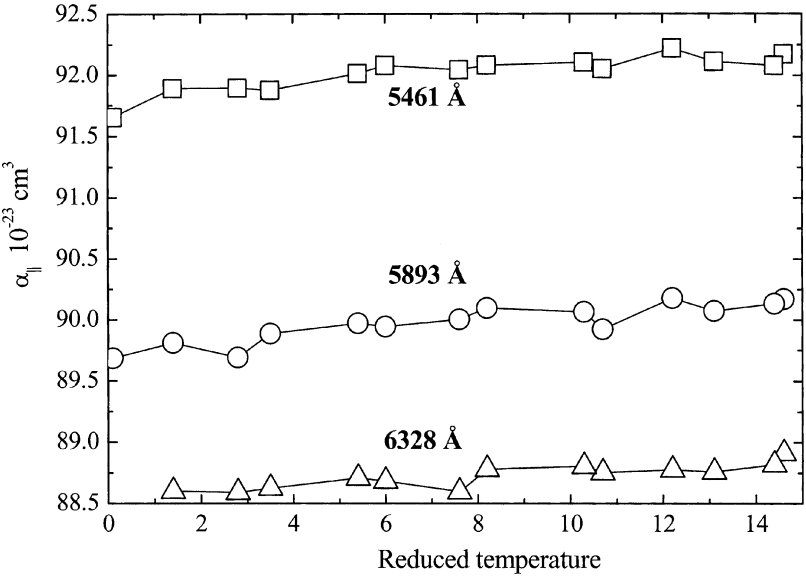

FIGURE 2 Polarisability tensor component $\alpha_{\parallel}\ 10^{-23}\,\mathrm{cm}^3$ of a CB 5 molecule as a function of the reduced temperature and the wavelength of the light.

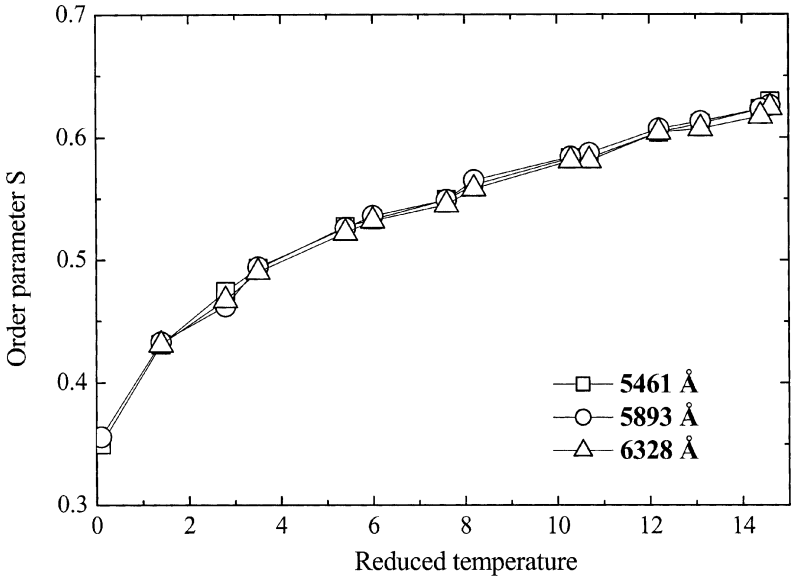

FIGURE 3 Order parameters S of a CB 5 liquid crystal as a function of the reduced temperature.

$(\alpha_{\parallel} - \alpha_{\perp})$ values. The change of wavelength for about 867 Å causes the change of polarisability anisotropy $(\alpha_{\parallel} - \alpha_{\perp})$ of about 2.48 10^{-23} cm^3 (see Fig. 1). The similar tendency in the relation to wavelength is correct because the commonly known phenomenon usually called as the refractive dispersion characteristic for the polarisability tensor components $\alpha_{\parallel}$ and $\alpha_{\perp}$ is investigated. Recall, that the refractive indices of all chemical substances are dependent on the wavelength of light. This fact influences the values of polarisability anisotropy $(\alpha_{\parallel} - \alpha_{\perp})$ and polarisability tensor components $\alpha_{\parallel}$ and $\alpha_{\perp}$. Another quantity characterising the liquid crystal molecule is the order parameter $S = (1/2)(3\cos^2 \Theta - 1)$.

Having the values of the coefficient k_A for the above mentioned wavelength, one can calculate the temperature dependence of the order parameter for these wavelengths. The values of order parameter S obtained for a CB 5 liquid crystal are listed in Tables 1–3, and illustrated additionally on Figure 3. A typical relation (see Fig. 3) between the order parameter S and reduced temperature was found for all wavelengths of the light. Thus, we confirmed that the order parameter S is not dependent on the wavelength of light. The result is correct as S describes the molecular arrangement in a liquid crystal sample. This fact confirms that the theory and its equations used in this work are correct as well. The same results were

TABLE 4 Relations of the Coefficient k_A, Polarisability Anisotropy $(\alpha_\parallel - \alpha_\perp)$ and $\alpha_\parallel$, $\alpha_\perp$ of a CB 5 Molecule and the Wavelength of the Light for Reduced Temperature Equal to 10.3°C

	ΔT	w.l. 5461 Å	w.l. 5893 Å	w.l. 6328 Å
k_A	10.3	3.0991	3.2097	3.2648
$(\alpha_\parallel - \alpha_\perp)$	10.3	42.95	40.95	40.14
$\alpha_\parallel$	10.3	92.11	90.07	88.81
$\alpha_\perp$	10.3	49.46	49.09	48.67

obtained for a CB6 liquid crystal for relations between the polarisability tensor components, the order parameter S and reduced temperature in the literature [12]. We wanted to say, in particular, that the correctness of the new relation between refractive indices and polarisability tensor component α was confirmed. This relation has the form of $(n^2 - 1) = (N\,d\,\alpha)/M^2$ and is better than the Lorenz – Lorentz equation $(n^2 - 1)/(n^2 + 2) = (N\,d\,\alpha)/M$. In Table 4, the relation between polarisability tensor components $\alpha_\parallel$ and $\alpha_\perp$, polarisability anisotropy $(\alpha_\parallel - \alpha_\perp)$, coefficient k_A, and the wavelength of the light is illustrated. It was determined that all these quantities are dependent on the wavelength of the light. Thus, during our study of the physical properties of liquid crystal molecules the attention to the "new parameter" like the wavelength of the light should be paid. It was also found that each wavelength of the light is characterised by new values of the coefficient k_A as a new parameter of physical properties of a liquid crystal molecule.

4. CONCLUSIONS

The main conclusions are the following:

- It was confirmed that all the quantities which are characterising the physical properties of a liquid crystal molecule, namely $\alpha_\parallel$, $\alpha_\perp$, and $(\alpha_\parallel - \alpha_\perp)$ are depended on the wavelength of the light.
- The changes of $\alpha_\parallel$ or $\alpha_\perp$ with the wavelength of light are not very large. It is about $3\ 10^{-23}\,cm^3$ for the change of the wavelength of the light from 6328 Å to 5461 Å which gives about 5% for $\alpha_\perp = 56.43\ 10^{-23}\,cm^3$. These changes are relatively large compared to the accuracy in calculation of $\alpha_\perp$ which are about $0.08\ 10^{-23}\,cm^3$.
- The investigation of the order parameter S of a CB 5 (p-cyano-p′-pentylbiphenyl) molecule confirms that this quantity is not dependent on the wavelength of the light. The order parameter S equals

$(\alpha_1 - \alpha_2)/(\alpha_\parallel - \alpha_\perp)$ which means that the change of $(\alpha_1 - \alpha_1)$ of a liquid crystal molecule is proportional to the change of refractive anisotropy $(n_e - n_o)$.

- The independence of the order parameter S on the wavelength of light proves the correctness of the theory and equations used in this calculation, in particular, the relation between refractive indices and polarisability tensor components α_1 and α_2 of the liquid crystal sample.
- It was found that the coefficient k_A is a function of the wavelength of light.
- Finally, it can be mentioned that all the results, namely the dependences of the polarisability tensor components and polarisability anisotropy on the wavelength of light, are in a very good agreement with the analogous study done on CB 6 molecule [12].

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