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Abstract. The orienting effect of a magnetic field on an erbium-based liquid crystal complex was studied by a capacitance method. The dependence of the effective dielectric permittivities of the complex on the magnetic field is obtained. A theoretical approach and a numerical method for determining the Frank elastic constants are proposed based on the experimental dependence of the effective values of the permittivity on various magnetic fields.

1. Introduction

The object of the study was a new mesogenic complex of tris [1- (4- (4-pentylcyclohexyl) phenyl) octane-1,3-dionato] - [5-heptadecyl-5'-methyl-2,2'-bipyridine] erbium. This $Er(DDk_{3\text{-}5})_3Bpy_{17\text{-}1}$ complex was synthesized at the Kazan National Research Technological University [1]. The chemical structure of the material under investigation is shown on the Figure 1. The erbium complex forms a nematic liquid crystal phase in the temperature range 130–160°C.

For the substance under study, the dependence of the effective dielectric permittivities on the value of the orienting magnetic field H is obtained.

Based on this dependence, the Frank elastic constants for the erbium complex are found by a numerical method.

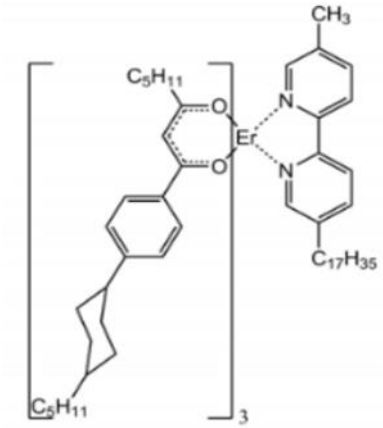

Figure 1. The chemical structure of the erbium liquid crystal complex

2. Methods

The proposed numerical method consists of two stages. First, a search is made for the minimum free energy of the liquid crystal cell [2,3]

$$F = S\int_0^d dz\,\omega(z)$$

where the free energy density has the form

$$\omega = \frac{1}{2}\left[(K_{11}\sin^2\theta + K_{33}\cos^2\theta)(\theta')^2 \mp \Delta\chi H^2\sin^2\theta - \frac{\Delta\varepsilon}{4\pi}\frac{U^2 d\cos^2\theta}{\int_0^d(\varepsilon_\perp + \Delta\varepsilon\cos^2\theta)^{-1}dz}\right]$$

As the boundary conditions, we consider models of strong and weak anchoring (the Rapini-Papoular potential) with different conditions of the pretilt at the boundaries. Here, the "–" or "+" sign corresponds to the magnetic field H perpendicular or parallel to the measuring electric field. The inhomogeneity of the electric field inside the sample is taken into account in both models.

At the second stage, the inverse problem of finding the Frank elastic constants K_{11} and K_{33} is solved by minimizing the deviation using the least squares method [4].

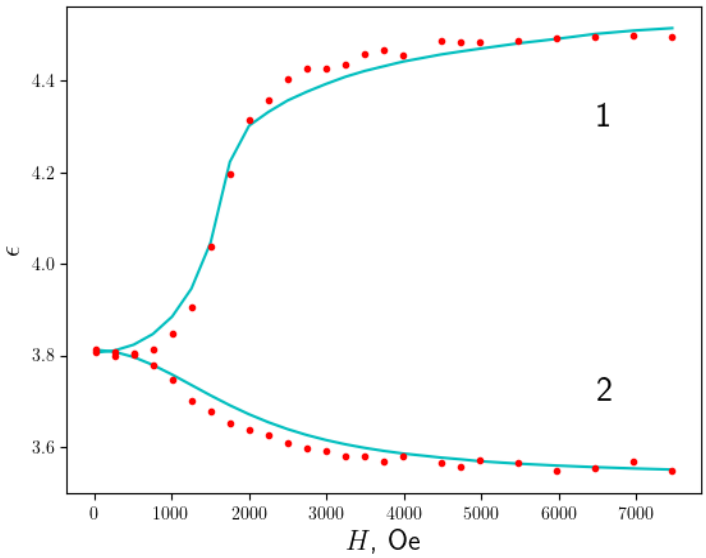

Figure 2. The dependence of the effective dielectric permittivity of the sample on the applied magnetic field (the direction of the magnetic field is 1 – parallel and 2 - perpendicular to the direction of the measuring electric field): experimental data (points) and calculation results (solid lines)

Figure 2 shows the experimental and theoretical dependences of the effective dielectric permittivity of the sample on the applied magnetic field, illustrating the results of our study. The match between the calculated and experimental data shows that the proposed method allows to achieve high accuracy using a small amount of experimental data. This statement is supported by an error estimation study.

This study consisted of three parts: first of all, it was necessary to evaluate the ability of the method to find a minimum on data without noise. For this, assuming K_{11} and K_{33} to be fixed, the theoretical dependence of the dielectric constant of the sample on the magnetic field was determined. Then we assumed that K_{11} and K_{33} were unknown. After that K_{11} and K_{33}, corresponding to the minimum deviation using the least squares method, were determined from the obtained dependence. Thus, it was found that on synthetic data the method can give accuracy up to the fourth digit. The second step was to test the method on a liquid crystal, for which the Frank constants are well known. A widespread 5CB liquid crystal was used as such an object. For 5CB, the values of K_{11} and K_{33} were calculated. They coincided with the values obtained by experimental methods with an accuracy of 5%.

In the final part of the study, using the described method, the Frank constants K_{11} and K_{33} were determined for the erbium complex and their errors were estimated:

$$K_{11} = (7 \pm 6)\ 10^{-6}\ \text{dyn},\ K_{33} = (6.7 \pm 0.5)\ 10^{-4}\ \text{dyn}.$$

3. Conclusions

As one can see, this method cannot provide accurate information about the K_{11} constant for the erbium complex, but at least the method gives us information that the K_{11} constant is several times smaller than K_{33}. The proposed method does not have such high accuracy as, for example, optical methods, but may be useful for some special cases when other more precise methods turn out to be inapplicable. It should be noted that the values of the Frank elastic constants for the erbium complex turned out to be quite large compared to ordinary liquid crystalline compounds.

4. References

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