Dielectric Technique to Measure the Twist Elastic Constant of Liquid Crystals: The Case of a Bent-Core Material

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Dielectric technique to measure the twist elastic constant of liquid crystals: 
The case of a bent-core material

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The effect of director pretilt on the twist magnetic Fréedericksz transition of nematics was investigated in a planar cell. The director configuration was calculated as a function of magnetic inductance. The dielectric and optical response of the nematic liquid crystal was numerically modeled. A dielectric measurement method for determining the elastic constant \( K_{22} \) is presented. The influence of the conditions for the Mauguin effect is discussed. The theoretical predictions were confirmed by our experiments. Experimental data for all elastic constants of a bent-core nematic material are presented and discussed.

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I. INTRODUCTION

The precise knowledge of material parameters is always valuable information for both applied and basic research. It helps to further improve or develop devices for industrial or scientific purposes and serves as input data for each and every phenomenon to understand, while the anomalous behavior of the parameters can refer to a novel effect or can be itself a phenomenon to understand.

Elasticity is one of the most common characteristics of liquid crystals. In nematic liquid crystals, there are three independent types of director deformation (splay, twist, bend) with the corresponding elastic constants \( K_{11}, K_{22}, K_{33} \), respectively [1]. Naturally, most liquid crystalline phenomena are strongly affected by elasticity. However, only a few effects are in practice used to measure the elastic constants due to precision issues.

The determination of \( K_{11} \) and of \( K_{33} \) is relatively simple by studying Fréedericksz transitions induced by electric and magnetic fields in different geometries [1–3]. With the help of numerical simulation and fitting methods, several material parameters (including \( K_{11}, K_{33} \), and the diamagnetic anisotropy \( \chi_0 \)) can be easily obtained from optical transmittance and by dielectric measurements in applied magnetic and electric fields, in the so-called splay geometry using a single planar cell [3].

Determining \( K_{22} \) in a similar way in the so-called twist-Fréedericksz geometry using a planar cell is much less trivial due to the problems discussed below, thus there were different other techniques employed. There were attempts to determine the Fréedericksz threshold by measuring birefringence in a planar cell using obliquely incident light [4,5] or applying electric and/or magnetic fields on a twisted nematic cell [6–8]. Other optical methods were also developed including conoscopic techniques [9–11], half leaky guided wave measurements [12], and methods based on light scattering [13–19]. Other techniques used cells with special in-plane electrodes [20–24]. Further experiments were carried out on wedge [25,26] and \( \pi \) cells [27]. \( K_{22} \) could also be determined in a torsion pendulum experiment in magnetic field [28].

In the twist-Frédéricksz geometry, the problems mentioned above affect both the optical transmittance and dielectric techniques. Due to the Mauguin effect, the polarization of the light follows the director and passes the cell almost unaffected under certain conditions [1,2]. The deformation thus can be detected only by measuring the depolarization occurring due to the failure of that conditions. In the present paper, we study these conditions for the Mauguin effect with a simulation technique, and we present our suggestions on how to overcome this problem during measurements.

Considering an ideal planar cell with indium tin oxide (ITO) electrodes on the glass substrates, no change in the capacitance due to twist deformation is expected. It will be shown, however, that this latter anticipation is not true in the presence of pretilt. We present a dielectric technique to measure \( K_{22} \) in a standard planar cell, which is, in several aspects, more versatile than the optical methods. We note that our technique differs from the dielectric method published in Ref. [20], which requires specially designed cells for the measurements.

Bent-core liquid crystals (BCs) are the subject of numerous studies currently, because of their fascinating features. The
reduced molecular symmetry of BCs compared to that of rodlike materials gave rise to many discoveries. Nonconventional, so-called banana phases were found \((B_1, B_2, \ldots, B_3)\) with unique properties (e.g., macroscopic chirality formed by achiral molecules [29]). Bent-core nematics (BCNs) are also in the focus of the research interest. Dielectric properties [30], flexoelectricity [31,32], pattern formation [33–37], and the presence of smectic clusters or cybotactic groups [38–40] are widely studied areas in BCNs. Anomalous elasticity of BCNs was published recently by several groups [3,41–43]. There seem to be general tendencies in the magnitudes and ratios of elastic constants in the case of BCNs. The magnitudes of \(K_{22}\) and \(K_{33}\) were found to be unusually small compared to rodlike nematics. The small \(K_{22} : K_{11}\) and \(K_{33} : K_{11}\) ratios were attributed to the presence of possibly chiral smectic clusters and the favorable bend distortion originating in the bent shape of the molecules.

In this paper we report about studies on the magnetic Fréedericksz transition in the presence of a director pretilt, and present the measurements of all Frank elastic constants of a cell with alignment layers rubbed antiparallelly. The this condition is a realistic assumption for the description of a cell with alignment layers rubbed antiparallelly. The pretilt angles should be the same at the two bordering surfaces.

The paper is organized as follows. In Sec. II the details of the theoretical description of the twist-Frédéricksz transition can be found. In Sec. III the results of our numerical calculations are shown and discussed. In Sec. IV our experimental technique is introduced. In Sec. V the results of the elastic constant measurements on a bent-core material are presented and compared with our calculations. Finally, in Sec. VI we summarize the results obtained.

II. THEORETICAL CONSIDERATIONS

A nonzero angle between the director and the alignment layer at the surface is called the pretilt. We consider a planar cell with strong anchoring and a pretilt of \(\Theta_0\), filled with a nematic liquid crystal with positive diamagnetic anisotropy \((\chi_d > 0)\). To achieve an undistorted initial director profile, the pretilt angles should be the same at the two bordering surfaces. This condition is a realistic assumption for the description of a cell with alignment layers rubbed antiparallelly. The geometry of the system can be seen in Figs. 1(a)–1(b). The film thickness is denoted by \(d\). The initial undistorted director field is perpendicular to the \(y\) direction. Homogenous magnetic inductance \(B = (B_x, B_y, B_z)\) is applied in a general direction. The magnitude of the field is denoted by \(B = |B|\). The pure twist geometry, however, corresponds to \(B_x = B_z = 0\). For simplicity we will use this case unless it is noted otherwise. Nevertheless our model can handle magnetic fields lying along a general direction. We will utilize this later when describing the case where \(B\) is slightly tilted from the \(y\) direction. In that way our model is more realistic to explain the effect of improperly adjusted geometry in the experiments.

With no pretilt, a magnetic inductance exceeding the threshold value \(B_{th}\) induces the twist-Fréedericksz transition, where the director profile can be described with one variable: the twist angle \(\phi\). In the presence of a director pretilt, a second variable, the tilt angle \(\Theta\) is also necessary for a complete description of the director field. The director components expressed by the two angles are

\[
\mathbf{n} = (\cos \Theta \cos \phi, \cos \Theta \sin \phi, \sin \Theta) .
\]

The torques acting on the director in a magnetic field lead to a change of both \(\phi\) and \(\Theta\). The deformation is homogenous, both angles depend only on the \(z\) coordinate. We assume that the cell is symmetric, therefore the maximum deformation occurs in the midplane (at \(z = d/2\)).

The total free energy density is the sum of the elastic and of the magnetic components:

\[
f_{\text{free}} = f_{\text{el}} + f_{\text{magn}},
\]

\[
f_{\text{el}} = \frac{1}{2} K_{11} (\nabla \mathbf{n})^2 + \frac{1}{2} K_{22} [\mathbf{n}(\nabla \times \mathbf{n})]^2
\]

\[
+ \frac{1}{2} K_{33} [\mathbf{n} \times (\nabla \times \mathbf{n})]^2 ,
\]

\[
f_{\text{magn}} = -\frac{1}{2} \frac{\chi_m}{\mu_0} (\mathbf{n} \mathbf{B})^2 .
\]

Plugging in the director profile of Eq. (1), we get

\[
f_{\text{free}} = \frac{1}{2} f(\Theta) \phi^2 + \frac{1}{2} f(\Theta) \phi^2 - \frac{1}{2} \frac{\chi_d}{\mu_0} \left[ B_x^2 \cos^2 \Theta \cos^2 \phi + B_y^2 \cos^2 \Theta \sin^2 \phi + B_z^2 \sin^2 \Theta + 2 B_x B_y \cos^2 \Theta \sin \phi \cos \phi + 2 B_x B_z \sin \Theta \cos \Theta \cos \phi + 2 B_y B_z \sin \Theta \cos \Theta \sin \phi \right],
\]

where prime refers to derivation with respect to \(z\) and

\[
f(\Theta) = K_{11} \cos^2 \Theta + K_{33} \sin^2 \Theta ,
\]

\[
g(\Theta) = \cos^2 \Theta (K_{22} \cos^2 \Theta + K_{33} \sin^2 \Theta) .
\]

We use Euler-Lagrange equations to minimize the free energy to obtain the equilibrium solutions for \(\Theta(z)\) and for \(\phi(z)\):

\[
\frac{d}{dz} \left( \frac{\partial f_{\text{free}}}{\partial \Theta'} \right) - \frac{\partial f_{\text{free}}}{\partial \Theta} = 0 ,
\]

\[
\frac{d}{dz} \left( \frac{\partial f_{\text{free}}}{\partial \phi'} \right) - \frac{\partial f_{\text{free}}}{\partial \phi} = 0 .
\]

After combining Eqs. (6)–(9), one arrives to a set of two second-order coupled nonlinear ordinary differential equations. This is a boundary value problem, with the mixed boundary conditions: \(\Theta(0) = \Theta_0\), \(\phi(0) = 0\), \(\Theta'(d/2) = 0\), and \(\phi'(d/2) = 0\). The numerical solution of the equations was provided by a MATLAB program.
The changes in the director field are usually monitored by dielectric or optical techniques. A later comparison with experiments thus requires the calculation of the cell capacitance and its optical transmittance. As the cell is inhomogeneous in the z direction, it is first split into thin slabs of thickness \( dz \) as shown in Fig. 2. The cell capacitance \( C \) is the net of the capacitances of all slabs connected in series. In the \( dz \rightarrow 0 \) limit one obtains

\[
C = C_0 \varepsilon_	ext{eff} = C_0 d \left( \int_0^d \frac{1}{\varepsilon_i + \varepsilon_a \sin^2 \Theta(z)} \, dz \right)^{-1}, \tag{10}
\]

where \( C_0 \) is the capacitance of the empty cell, \( \varepsilon_	ext{eff} \) is an effective, \( \varepsilon_i \) is the perpendicular dielectric constant, and \( \varepsilon_a \) is the dielectric anisotropy.

The optical response of the cell has been calculated with the Mueller-matrix method [44–46]. A (partially) polarized light can be described by a four-element Stokes vector. Its definition and an example of a Stokes vector for light linearly polarized can be described by a four-element Stokes vector. Its definition in Eq. (10) for \( 0 < B < 5B_{th} \) in two cases: the first is the

\[
\mathbf{s}_{\text{out}} = \mathbf{M}_{\text{pol}}(\alpha_p) \left( \prod_{i=1}^{n} \mathbf{M}_{wp}(\phi_i, \Delta \phi_i) \right) \mathbf{M}_{\text{pol}}(\alpha_p) \mathbf{s}_{\text{in}}. \tag{12}
\]

The optical transmittance is given by the ratio of the first elements of \( \mathbf{s}_{\text{out}} \) and of \( \mathbf{s}_{\text{in}} \). \( \mathbf{s}_{\text{in}} \) was chosen to be linearly polarized in the direction of \( \alpha_p \) (parallel to the polarizer).

We set \( \alpha_p = 0 \) and \( \alpha_a = 90^\circ \), thus the optical transmittance is proportional to the expected depolarization.

### III. Simulation Results and Discussion

During simulations the magnetic inductance values were counted in units of \( B_{th} = \frac{\mu_0 H_0}{|\mu_0|} \), which is the Fréedericksz threshold inductance for the twist geometry with zero pretilt. All the simulations were performed using the material parameters of 5CB [3]. A pretilt of \( \Theta_0 = 2^\circ \) was assumed. Figures 3a–3b show the change in the calculated twist and tilt angles inside the sample for three different magnetic inductances. Below the threshold, at \( B/B_{th} = 0.5 \), there is no deformation, \( \phi \) remains zero while \( \Theta(z) = \Theta_0 \). Above the threshold the twist angle increases, while the tilt angle decreases, just as it was expected. At higher inductances, \( \phi \) approaches \( 90^\circ \), while \( \Theta \) goes to 0 far from the substrates.

We define \( \beta \) as a small misalignment angle of \( \mathbf{B} \) from the y direction in the y-z plane, thus \( \tan \beta = B_z/B_y \) (and \( B_z = 0 \)). We have calculated the effective permittivity \( \varepsilon_{\text{eff}} \) defined in Eq. (10) for \( 0 < B < 5B_{th} \) in two cases: the first is the

\[
\Delta \phi_i = \frac{2\pi}{\lambda} \left( \frac{n_e}{1 + \frac{n_e^2 - n_o^2}{n_o^2} \sin^2 \Theta_i} - n_o \right) dz, \tag{11}
\]

where \( \lambda \) is the wavelength of light, \( n_o \) and \( n_e \) are the ordinary and extraordinary refractive indices of the liquid crystal, respectively, while \( \Theta_i \) is the tilt angle at the position of the \( i \)th slab. The Mueller matrix of the \( i \)th slab of our liquid crystal cell is \( \mathbf{M}_{wp}(\phi_i, \Delta \phi_i) \). We also introduce \( \mathbf{M}_{\text{pol}}(\alpha) \), the Mueller matrix of a polarizer placed at an angle \( \alpha \) with respect to the x direction in our geometry. The matrices can be found in the Appendix. The liquid crystal cell is placed between polarizers. The angles of the polarizer and analyzer are \( \alpha_p \) and \( \alpha_a \), respectively. If the cell is illuminated with an incident monochromatic light with a Stokes vector of \( \mathbf{s}_{\text{in}} \), the

\[
\mathbf{s}_{\text{out}} = \mathbf{M}_{\text{pol}}(\alpha_a) \left( \prod_{i=1}^{n} \mathbf{M}_{wp}(\phi_i, \Delta \phi_i) \right) \mathbf{M}_{\text{pol}}(\alpha_p) \mathbf{s}_{\text{in}}. \tag{12}
\]

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perfectly aligned geometry with pretilt ($\Theta_0 = 2^\circ$ and $\beta = 0^\circ$), the other is a misaligned case with no pretilt ($\Theta_0 = 0^\circ$ and $\beta = 2^\circ$). As $\varepsilon_{\perp} < \varepsilon_{\text{eff}} < \varepsilon_{||}$ always fulfills for liquid crystal samples with $\varepsilon_a > 0$, for the visualization of the magnetic field dependence of $\varepsilon_{\text{eff}}$ it is convenient to plot the reduced quantity $(\varepsilon_{\text{eff}} - \varepsilon_{\perp})/\varepsilon_{\perp}$, as presented in Fig. 4 (solid and dashed lines for the two cases correspondingly).

It is important to emphasize at this point that without a director pretilt ($\Theta_0 = 0^\circ$) in a perfectly aligned geometry ($\beta = 0^\circ$) no change is expected in $\varepsilon_{\text{eff}}$ as it does not depend on $\phi$. If we have $\Theta_0 \neq 0^\circ$ in Fig. 4, however, a Fréedericksz transition with sharp threshold behavior can clearly be seen. The sharp transition is owing to the fact that the initial director is perpendicular to $B$ even in the presence of a pretilt, in contrast to the splay geometry (see Fig. 10), where the pretilt makes the threshold smooth. This effect thus gives us a dielectric measurement technique to study the twist-Fréedericksz transition and use it to determine $K_{22}$. This technique could be widely applied, because a small, well defined pretilt is always present as a consequence of the rubbing of a planar polyimide alignment layer. The threshold inductance value is seemingly very close to $B_\text{th}$ defined before, which can be expected for the case of a small pretilt. Below the threshold $\varepsilon_{\text{eff}} = \varepsilon_{\perp} + \varepsilon_a \sin^2 \Theta_0$, while towards high inductances it converges to $\varepsilon_{\perp}$. The maximum change of $\varepsilon_{\text{eff}}$ is thus in the order of 0.1% of $\varepsilon_a$ for usual pretilts. This is a small value, especially for compounds with low dielectric anisotropy, however, a good capacitance bridge has a resolution in the order of parts per million (or better), so is more than capable of performing such measurement.

A change of $\Theta$ also occurs at no pretilt if the magnetic field has a small misalignment (Fig. 4, dashed line). Here the magnetic field is also perpendicular to the initial director, thus we can see a sharp transition. The change in the effective dielectric constant here is due to the presence of $B_c \neq 0$ and is of the same order of magnitude as in the pretilt case. The relative change has, however, an opposite sign. In the more realistic case where both $\Theta_0 \neq 0^\circ$ and $\beta \neq 0^\circ$, the two effects counteract together reducing the change in $\varepsilon_{\text{eff}}$. Furthermore the transition is expected to be less sharp, because $B$ is then not perpendicular to the initial director. As a consequence, misalignment of the field should be avoided in an experiment in order to obtain precise data. This can be achieved by using a sample holder with appropriate geometrical constraints with respect to the poles of the magnet.

Calculation of the director field also allows the study of the optical behavior of the cell. It is well known that the adiabatic light propagation along a cholesteric helix requires the Mauguin condition, $\lambda \ll P n_a$ to satisfy ($P$ is the helical pitch, and $n_a = n_e - n_o$ is the optical anisotropy) [1]. In our twist-Fréedericksz geometry the gradient of the twist angle, $\phi'$, plays the role of the wave number of the helix, thus the above condition is the equivalent of $\lambda \ll M_0 n_e$. It is convenient to introduce a dimensionless quantity, $\eta = \pi \varepsilon_{\perp}/\varepsilon_{\text{max}} n_e$ as a measure of how well the Mauguin condition (1 $\ll \eta$) fulfills [max($\phi'$) is the maximal value of $\phi'(z)$ in the cell]. As $\eta$ decreases, one gradually leaves the adiabatic light propagation regime, thus the depolarization of the transmitted light becomes stronger. Though this is a continuous transition, for a qualitative analysis of the dependence on magnetic inductance, pretilt angle and cell thickness it is convenient to choose an arbitrary large number (e.g., $\eta = 20$) as a discriminating value. Then one can (approximately) say that being in the Mauguin limit corresponds to $\eta > \eta_c$.

In our geometry the twist is induced by the magnetic inductance. Figure 5 shows $\eta$ versus $B/B_{\text{th}}$ calculated for a $d = 30 \, \mu\text{m}$ thick cell assuming different pretilt angles. The monotonic decrease of $\eta(B/B_{\text{th}})$ means that the higher the magnetic inductance above $B_{\text{th}}$, the less adiabatic the light propagation through the cell. This is due to the increasing $\phi$ gradients near the substrates as seen also in Fig. 3(a). One can formally introduce a critical magnetic inductance $B_c$ with $\eta(B_c) = \eta_c$. For $B/B_{\text{th}} > B_c$ one is outside the Mauguin limit, therefore strong depolarization is expected. For $B/B_{\text{th}} < B_c$, however, light propagates adiabatically, therefore depolarization is small; the measurement of depolarization might not be sensitive enough for studying the Fréedericksz transition.

Figure 5 shows that the $\eta(B/B_{\text{th}})$ curves and thus $B_c$ shifts toward higher $B/B_{\text{th}}$ values if a director pretilt is introduced (i.e., the pretilt reduces the $\phi$ gradients).

Figure 6 exhibits the thickness dependence of $B_c$. It is seen that the growth of $B_c$ with $d$ is substantial. This implies that the proper choice of the cell thickness is really
important for studying the twist-Fréedericksz transition by optical depolarization measurements; low thickness with low pretilt gives the best results. We should emphasize, however, again that \(\eta_c\) and \(B_c\) are not real thresholds, but just helpful tools to obtain the conclusions above purely from knowing the director field in the cell.

Calculation of the actual optical transmittance confirmed the tendencies concluded in the previous paragraph. Figure 7 depicts the magnetic inductance dependence of the transmittance in cells of different thicknesses, but without pretilt, under the conditions of crossed polarizers, with the polarizer parallel with the initial director. It is evident that the transition is much sharper and the transmittance is much larger in a thinner cell. We can conclude that the optical measurement problems described in Ref. [2] are actually present only for thicker cells; the technique works well for thin cells, though there higher magnetic inductances are needed. Nevertheless, moderate \(B \sim 1\) T inductances may be sufficient (e.g., for a 10 \(\mu\)m thick planar cell filled with 5CB: \(B_{th} = 0.6\) T).

When a director pretilt is present, both the twist and the tilt angles change with the applied field. Consequently the transmitted light intensity depends, besides the depolarization, on the birefringence variation too. This is demonstrated in Fig. 8, which presents the calculated transmittance of a \(d = 30\) \(\mu\)m cell for three different pretilt values. The main feature of this plot is the appearance of a hump at the highest pretilt, which we attribute to the effect of birefringence. We note that at higher thickness and pretilt values, the intensity oscillations strongly depend on the parameters of the cell (e.g., thickness, material constants), thus the interpretation of a measurement curve is rather difficult. This is another argument for the use of thin cells.

**IV. EXPERIMENTAL TECHNIQUE**

In order to demonstrate the usability of the dielectric method to determine \(K_{22}\), we have prepared an experiment on the well known compound 4'-pentyl-4-cyanobiphenyl (5CB). Experiments on a different setup have been carried out on the bent-core material abbreviated as DT6PY6E6 [47] (Thiadiazol with a pyridine arm with two hexyloxy chains and an ester arm with two lateral hexyloxy chains. The ethyl ester is connected via a hexamethylene spacer.). Its chemical structure is shown in Fig. 9.

The synthesis and the molecular properties of the compound have been published recently [47]. DT6PY6E6 has a nematic phase in a relatively wide temperature range. The clearing point is \(T_{NI} = 149\) °C, the melting point is at 93 °C in heating, while the nematic phase can be supercooled down to room temperature.

The different custom made sandwich cells with ITO electrodes were filled with 5CB and with DT6PY6E6 in the isotropic phase. The thickness of the empty cells were \(d = 26\) \(\mu\)m and \(d = 27.3\) \(\mu\)m, respectively. \(d\) was measured by interferometry. Rubbed polyimide was used as alignment
In the splay geometry the polarizer was adjusted to 45° with respect to the initial director to get the highest intensity, while this angle was set to zero in the other case, where only the depolarization had to be measured.

Both measurement systems were automatized and controlled by LABVIEW programs.

V. EXPERIMENTAL RESULTS AND DISCUSSION

The magnetic inductance dependence of $\varepsilon_{\text{eff}}$ in the twist geometry for 5CB at $T_{N1} - T = 8^\circ\text{C}$ is presented in Fig. 11.

The best numerical fit of the dielectric data is shown by the solid line. (The following material constants used by the fit were taken from the literature: $K_{11} = 5.9$ pN and $K_{33} = 10$ pN [19], $\varepsilon_{||} = 17.5$ [48], and $\chi_a = 1.2 \cdot 10^{-6}$ [49].) From the threshold inductance (see dotted line) we have $K_{22} = 4.2$ pN, which is close to the literature value of $K_{22} = 3.9$ pN [19]. The fit value of the pretilt is $\Theta_{\parallel} = 1.5^\circ$, which is realistic. Our data are moderately noisy, but they clearly show that the principle of the measurement is working and the measurements with adequate precision can be realized even with a regular oscilloscope. We have measured a decreasing effective dielectric constant during the transition, which means the change in $\varepsilon_{\text{eff}}$ originates dominantly from the presence of a pretilt.

The magnetic inductance dependence of $\varepsilon_{\text{eff}}$ and the voltage dependence of the optical phase difference $\Delta \Phi$ in the splay geometry for the compound DT6PY6E6 at $T = 125^\circ\text{C}$ are shown in Figs. 12 and 13, respectively.

The solid lines correspond to experimental data recorded with a high sample density. The dashed lines are numerical fits obtained using the numerical methods published in Ref. [3] to extract the material parameters from the experimental data. The quality of the fits are saliently good. We have determined the elastic constants: $K_{11} = 5.4$ pN, $K_{33} = 10$ pN; the diamagnetic anisotropy: $\chi_a = 7.4 \cdot 10^{-7}$; the dielectric constants: $\varepsilon_{\perp} = 4.1$, $\varepsilon_{||} = 5.9$; and the optical anisotropy: $n_a = 0.24$.

The magnetic inductance dependence of $\varepsilon_{\text{eff}}$ and of the transmitted intensity measured in the twist geometry in DT6PY6E6 is presented in Fig. 14 by solid and dash-dotted curves, respectively. The best numerical fit of the dielectric

FIG. 10. (Color online) The schematic figure of the splay-Fréedericksz transition geometry.

FIG. 11. (Color online) The magnetic inductance dependence of $\varepsilon_{\text{eff}}$ in the twist geometry for the compound 5CB at $T_{N1} - T = 8^\circ\text{C}$. The triangles are experimental data points. The solid line is numerical fit.
DIELECTRIC TECHNIQUE TO MEASURE THE TWIST

FIG. 12. (Color online) The magnetic inductance dependence of \( \varepsilon_{\text{eff}} \) in the splay-Frédéricksz transition for the compound DT6PY6E6 at \( T = 125 \, ^\circ \text{C} \). The solid line is experimental data. The dashed line is numerical fit.

data is shown by the dashed line. (The values of \( K_{33} \) and of \( \chi_a \) determined by the fit in the splay geometry were used here.) From the threshold inductance (see dotted line) we have \( K_{22} = 2.2 \, \text{pN} \). The optical intensity is more noisy than the dielectric data in spite of the fact that the relative change in the latter is in the order of 1/1000. It seems to be more difficult to locate the threshold by the optical method. Comparing this measurement with the one prepared on 5CB, here also stands that due to the decrease in \( \varepsilon_{\text{eff}} \), the effect dominantly originates from the presence of pretilt. This dataset is much less noisy, because the precision of the capacitance bridge is much higher than that of the oscilloscope technique presented above.

The Frank elastic constant values of DT6PY6E6 do not follow the trends reported by independent authors [3,41–43] for bent-core compounds. The elastic constants of DT6PY6E6 can rather be considered as typical for rodlike liquid crystals. \( K_{22} \) is rather low, however, it is not as low (~0.3 pN) as for the BCN in Ref. [3]. The magnitude of \( K_{33} \) is large and \( K_{33}/K_{11} > 1 \).

We think that the non-BCN behavior of DT6PY6E6 might be due to the effect of the four alkyl chains connected to intermediate core rings. The alkyl chains can easily change conformation with relatively low energy cost (they are not rigid). They can act like soft spacers between molecules. Thus, for topological reasons, the chains might prevent the direct steric interaction between the rigid bent shaped cores in the nematic phase. Therefore the system looses its tendency to favor a polar packing, which has led to unusual properties via smectic cluster formation in other BCNs. This idea is in accordance with x-ray results on DT6PY6E6 [47]. The distance between molecules are unusually large, which could prevent the prevalence of the bent-core properties such as anomalous elasticity, due to the lack of strong core-core interactions.

We note that the presence of alkyl chains on the arms of the molecules can also affect the anchoring strength. In future studies this also could be investigated, for example, using the method worked out by Sugiyama et al. [50].

VI. SUMMARY

We have studied the magnetic twist-Frédéricksz transition in the presence of pretilt with numerical modeling. We showed, that the nonzero director pretilt offers a dielectric measurement method to obtain the \( K_{22} \) elastic constant. We have simulated the light propagation through the cell and determined the transmittance as a function of magnetic inductance with different thickness and pretilt values. It was found that higher pretilt can qualitatively change the the transmittance profile. This is in contrast to the monotonic increase expected in the zero pretilt case near the threshold, where the major effect originates only from the depolarization effect. It was proven that the Mauguin effect causes trouble only in case of thick cells; with the thickness around 10 \( \mu \text{m} \), the depolarization technique shows well the threshold values.

We have performed Frédéricksz-transition experiments in the splay and twist geometries to determine all the elastic constants of the BCN compound DT6PY6E6, using only a single planar cell. In the twist geometry, our theoretical considerations were confirmed by the measurements. We were able to determine \( K_{22} \) with the help of the dielectric method, which seems to be more versatile in many aspects than the conventional optical technique.

The elastic constants of DT6PY6E6 are found to be similar to that of rodlike materials. This is explained by the effect...

FIG. 13. (Color online) The voltage dependence of \( \Delta \Phi \) in the splay-Frédéricksz transition for the compound DT6PY6E6 at \( T = 125 \, ^\circ \text{C} \). The solid line is experimental data. The dashed line is numerical fit.

FIG. 14. (Color online) The magnetic inductance dependence of \( \varepsilon_{\text{eff}} \) (measured data: solid line, fit: dashed line) and of the transmitted intensity (dash-dotted line) measured on DT6PY6E6 in the twist geometry. The \( B_{th} \) threshold inductance determined by the fit is at the dotted line.
of intermediate alkyl chains, which could prevent strong core-core interactions between molecules and increase the intermolecular distance.

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APPENDIX

A monochromatic ray of light propagating along the z direction can be described by the x and y components of its electric field vector $E_x(z,t) = E_{0x} \cos(\omega t - k z)$, $E_y(z,t) = E_{0y} \cos(\omega t - k z + \delta)$, respectively [45]. ($\omega$, $k$, and $\delta$ are the angular frequency, the wave number, and the phase difference, respectively.) The Stokes vector is constructed as

$$ s = \begin{bmatrix} s_0 \\ s_1 \\ s_2 \\ s_3 \end{bmatrix} = \begin{bmatrix} E_{0x}^2 + E_{0y}^2 \\ 2E_{0x}E_{0y}\cos\delta \\ 2E_{0x}E_{0y}\sin\delta \\ 0 \end{bmatrix}. $$

For example, the Stokes vector for linearly polarized light in the x direction with the total intensity 1 is described by: $s_0 = 1$, $s_1 = 1$, $s_2 = 0$, and $s_3 = 0$.

The Mueller matrix of a birefringent slab with an optical phase difference of $\Delta \varphi$ is given by

$$ M_{\mu\varphi}(\varphi, \Delta \varphi) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos^2 2 \varphi + \cos \Delta \varphi \sin^2 2 \varphi & (1 - \cos \Delta \varphi) \sin 2 \varphi \cos 2 \varphi & \sin \Delta \varphi \sin 2 \varphi \\ 0 & (1 - \cos \Delta \varphi) \sin 2 \varphi \cos 2 \varphi & \sin^2 2 \varphi + \cos \Delta \varphi \sin^2 2 \varphi & -\sin \Delta \varphi \cos 2 \varphi \\ 0 & -\sin \Delta \varphi \sin 2 \varphi & \sin \Delta \varphi \cos 2 \varphi & \cos \Delta \varphi \end{bmatrix}, \quad (A2) $$

$\phi$ is the angle between the slow axis and the x direction in our geometry.

The Mueller matrix of a polarizer set in an angle of $\alpha$ with respect to the x direction in our geometry

$$ M_{pol}(\alpha) = \begin{bmatrix} 1 & \cos 2 \alpha & \sin 2 \alpha & 0 \\ \cos 2 \alpha & \cos^2 2 \alpha & \sin 2 \alpha \cos 2 \alpha & 0 \\ \sin 2 \alpha & \sin 2 \alpha \cos 2 \alpha & \sin^2 2 \alpha & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \quad (A3) $$


