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Dielectric Anisotropy Properties of BAC-Doped 5CB Liquid Crystal

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*Dielectric anisotropy properties and splay elastic constant, K_{11} for **5CB** (4-cyano-4'-pentylbiphenyl) plus 1% **BAC**(4-[4-(S)-2-methylbutoxybenzoyloxy]benzoic acid] have been investigated. The frequency dependent dielectric anisotropy and splay elastic constant have been calculated by using capacitance-voltage curves for various frequencies. The critical frequency, f_c values of dielectric anisotropy for 4-cyano-4′-pentylbiphenyl (**5CB**) and **5CB+(1%)BAC** composites were found to be 433.5 kHz and 439.5 kHz, respectively. It has been determined that **BAC** doping to **5CB** decreases both threshold voltages and splay elastic constants for all frequencies applied. The decrease in K_{11} values has been interpreted as the decrease of distortion in the system.*

Keywords 4-[4-(S)-2-Methylbutoxybenzoyloxy]benzoic liquid crystal acid; 5CB liquid crystal; dielectric anisotropy; splay elastic constant.

1. Introduction

The dielectric properties of a number of nematic liquid crystals have been investigated both experimentally and theoretically [1–3]. Nematic liquid crystals have also been extensively studied due to their extraordinary properties and their promising applications in recent technologies [4–9]. Dielectric spectroscopy method is used to obtain the valuable information about the molecular properties of nematic liquid crystals. This method has been found to be one of the best for the measurement of permittivity and dielectric loss with high accuracy and sensitivity [10,11]. Since liquid crystals composites with nematics have also attracted much attention over the years because of their electro-optic applications, there have been various works concentrating on the electro-optical characterization of LCs [12–17].

This paper reports the dielectric anisotropy properties of BAC doped **5CB** and **5CB+(1%)BAC** nematic liquid crystal. Thus, we have prepared a liquid crystal mixture of **5CB** and **5CB+(1%)BAC** to develop its dielectric anisotropy property and dielectric parameters for electro-optic applications.

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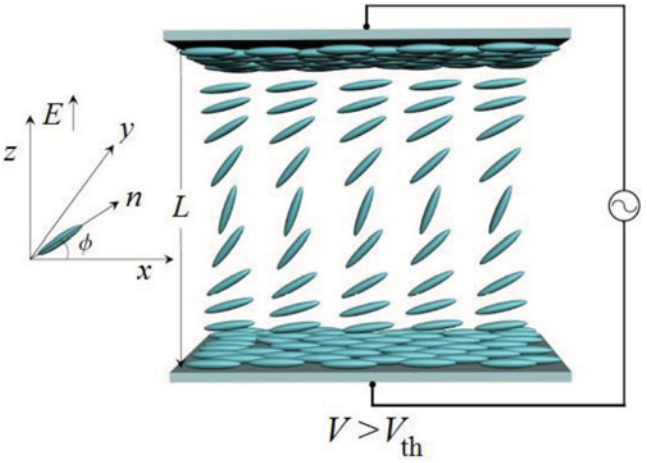


Figure 1. Change of orientation of the molecules with applied electric field [18].

2. Theoretical Background

The application of an electric field to liquid crystal system results a significant change in orientation of molecules depending on the value of the electric field inside (Fig. 1).

As the electric field (i.e., voltage applied) increases, at first no change in alignment of the molecules is observed. However, if a certain voltage value i.e., threshold voltage V_{th} is exceeded, the orientation of molecules starts to change from perpendicular to parallel with respect to electric field (Fig. 2). The occurrence of such a change from an aligned to a deformed state is called Fréedericksz transitions [19].

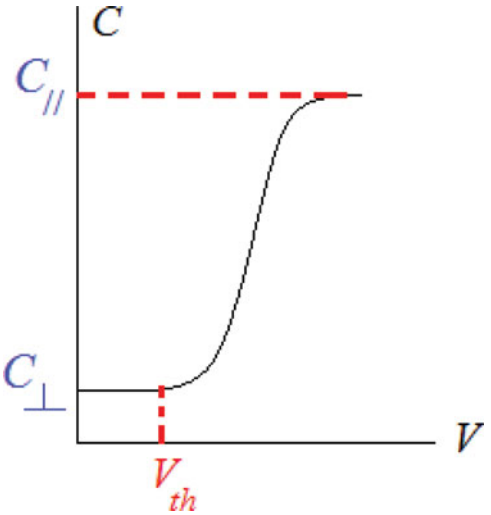


Figure 2. Determination of threshold voltage, V_{th}, by C-V graphics. ($C_{//}$ and $C_{\perp}$ denote the parallel and perpendicular capacitances, respectively.)

According to Fig. 2, the perpendicular and parallel dielectric constants ($\varepsilon_\perp$ and $\varepsilon_{//}$) are calculated by capacitance method.

$$C_\perp = \varepsilon_\perp \varepsilon_0 A/d \tag{1}$$

$$C_{//} = \varepsilon_{//} \varepsilon_0 A/d \tag{2}$$

The dielectric anisotropy for the liquid crystals is determined by the following relationship [20].

$$\Delta\varepsilon = \varepsilon_{//} - \varepsilon_\perp \tag{3}$$

Most liquid crystals have a permanent or induced dipole moment along or across the long molecular axis. The orientation of dipole moment determines the molecule orientation. If the dipole moment is parallel to the long molecular axis, $\Delta\varepsilon$ becomes positive and molecules tend to orient along the electric field direction (Fig. 3a). If the molecules carry dipole moments that are more or less normal to the long molecular axis, $\Delta\varepsilon$ becomes negative and molecules tend to orient perpendicular to the electric field direction (Fig. 3b) [21].

Under an external field, the total free energy of liquid crystal, F_T, is defined by the sum of free energy density of uniformly aligned state, F_o and distortion free energy density, F_d (Eq. 4)

$$F_t = F_0 + \frac{1}{2}K_{11}\left(\vec{\nabla} \cdot \hat{n}\right)^2 + \frac{1}{2}K_{22}\left(\hat{n} \cdot \vec{\nabla} \times \hat{n}\right)^2 + \frac{1}{2}K_{33}\left(\hat{n} \times \vec{\nabla} \times \hat{n}\right)^2 \tag{4}$$

where $\hat{n}$ is the normalized director of molecules of LC that describes the nature of distortion. K_{11}, K_{22}, and K_{33} are elastic constants with energy/length unit and they are typically in the order of pN. K_{11}, K_{22}, and K_{33} in Eq. (4) also represent a type of splay, twist, and bend distortions, respectively. A sum of these terms describes an arbitrary distortion of LC system. Equation (4) is valid for nematic LCs. In the case of chiral nematic LCs, Eq. (4) is modified by introducing q_0 parameter which is defined as $2\pi/P_0$ (P_0 is the pitch of cholesteric helix) [22].

$$F_t = F_0 + \frac{1}{2}K_{11}\left(\vec{\nabla} \cdot \hat{n}\right)^2 + \frac{1}{2}K_{22}\left(\hat{n} \cdot \vec{\nabla} \times \hat{n} + q_0\right)^2 + \frac{1}{2}K_{33}\left(\hat{n} \times \vec{\nabla} \times \hat{n}\right)^2 \tag{5}$$

The splay elastic constant, K_{11} is calculated by Eq. (6)

$$K_{11} = V_{th}^2 \varepsilon_0 \Delta\varepsilon/\pi^2 \tag{6}$$

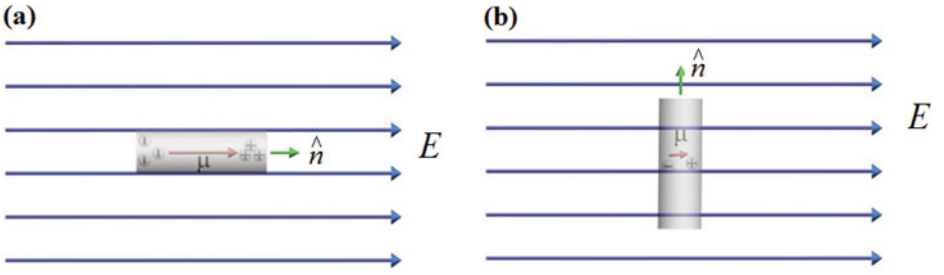
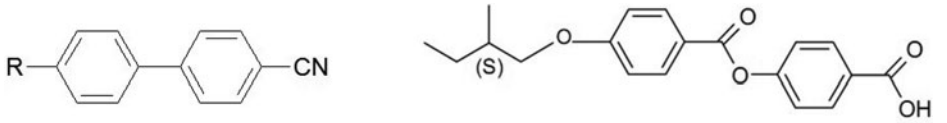


Figure 3. Liquid crystal molecules with **(a)** $\Delta\varepsilon > 0$ and **(b)** $\Delta\varepsilon < 0$ in electric field [21].



a) 5CB: R = C_5H_{11}; Cr 25 N 34 Iso **b) BAC**: Cr 168 N* 184 Iso

Figure 4. The chemical structures and phase transition temperatures of **(a) 5CB (**4-cyano-4′-pentylbiphenyl) and **(b) BAC (**4-[4-(S)-2-methylbutoxybenzoyloxy]benzoic acid).

3. Experimental

The preparation procedure, spectroscopic, and mesomorphic data for 4-[4-(S)-2-methylbutoxybenzoyloxy]benzoic acid (**BAC**) were already given in Refs. [23–26]. The transition temperatures were measured using a Linkam THMS 600 hot stage and a Linkam TMS 93 temperature control unit in conjunction with a Leitz Laborlux 12 Pol. polarizing microscope. The chemical structures of the **5CB** and **BAC** have been shown in Fig. 4.

Empty cells have been prepared by indium-tin-oxide (ITO) coated glass plates purchased by Instec Colorada Inc. (Fig. 5). The inner surfaces of the glasses have been coated with the aligning polyimide layers. The thickness of the empty cells was set as $d = 9 \pm 0.1\ \mu$m by Mylar spacer. The ITO cells have been filled with the **5CB** and **5CB+(1%)BAC** by capillary action.

The variation of capacitance with applied voltage measurements of **5CB** and **5CB+(1%) BAC** have been performed by HP 4192A LF Impedance Analyzer within the frequency range of 5 Hz–13 MHz. The LC cells were screened any electric field effects by Faraday cage. The schematic representation of the experimental system has been given in Fig. 6.

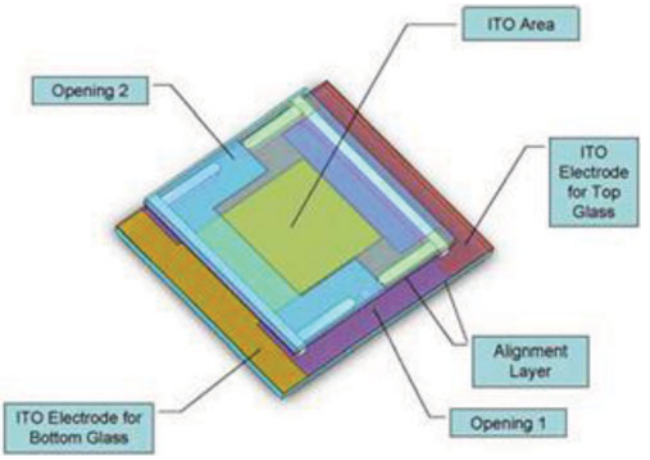


Figure 5. The structure of empty LC cell.

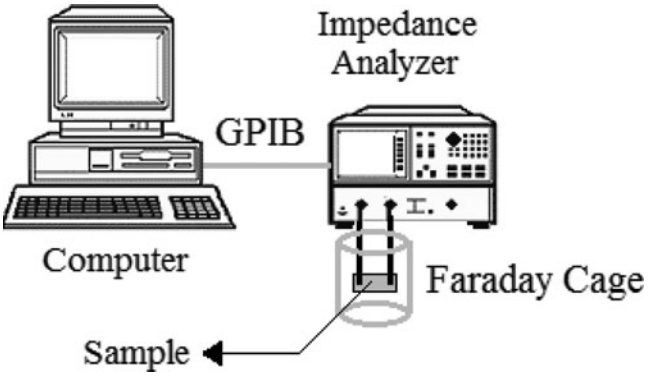


Figure 6. The schematic representation of the experimental setup.

4. Results and Discussions

4.1. Liquid Crystalline Properties of the BAC

The liquid crystal (**BAC**) phase sequence is given as follows:

$$\mathrm{Cr} \xrightarrow{168^{\circ}\mathrm{C}} \mathrm{N}^{*} \xrightarrow{184^{\circ}\mathrm{C}} \mathrm{Iso}$$

According to polarizing microscope studies, **BAC** chiral nematic material exhibits a thermotropic enantiotropic mesophase between 168°C and 184°C. The textures of **5CB** and **5CB+(1%)BAC** have also been shown in Fig. 7.

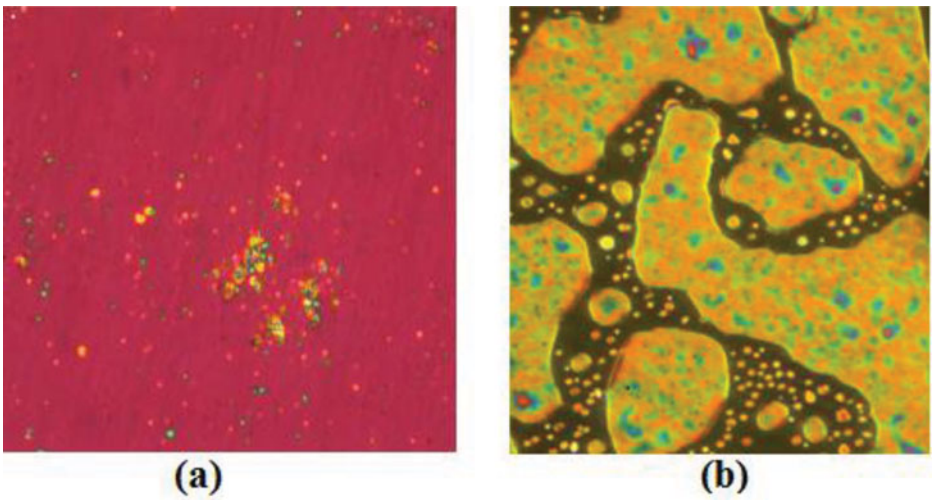


Figure 7. Polarized light optical photomicrographs of the **(a) 5CB** at 30°C **(b) 5CB+(1%)BAC** at 34.8°C (x200 Magnification).

Table 1. The threshold voltages and dielectric anisotropies for 5CB and 5CB+(1%)BAC at some selected frequencies

5CB	1 kHz	10 kHz	100 kHz	200 kHz
V_{th} (V)	21.65	13.73	19.59	15.27
$\Delta\varepsilon$	3.89	4.78	2.85	1.93
5CB+BAC (1%)	1 kHz	10 kHz	100 kHz	200 kHz
V_{th} (V)	4.56	3.61	2.89	0.98
$\Delta\varepsilon$	6.39	6.99	4.21	2.56

4.2. Dielectric Anisotropy Properties and Splay Elastic Constant of LC Composites

The capacitance-voltage characteristics of the liquid crystals under various frequencies have been given in Fig. 8a and Fig. 8b for **5CB** and **5CB+(1%)BAC**, respectively. As is seen in the figures, at lower voltages, the capacitance of the liquid crystals is almost constant and after a certain voltage, it increases drastically and reaches saturation due to molecular reorientation of the liquid crystals. This *C–V* characteristic is valid for the frequency interval of 1–400 kHz. Above 400 kHz, the capacitance of the liquid crystals is almost constant and after a certain voltage, it decreases and then reaches saturation. In this respect, it has been deduced that the orientations of molecules change their direction above 400 kHz.

The minimum value of the capacitance corresponds to original orientation of the molecules. Once the voltage applied is increased, the molecular orientation starts and in turn, the capacitance increases with voltage applied. The **5CB** liquid crystal has the highest Fréedericksz threshold voltage with respect to **5CB+(1%)BAC** composite (see Fig. 8c and 8d). This suggests that the **BAC** molecules have the high molecular orientation ability.

According to Fig. 8a and 8b, the parallel and perpendicular capacitance values have been determined for various frequencies. The perpendicular and parallel dielectric constants that correspond to perpendicular and parallel molecular orientations have been calculated by the capacitance method via Eqs. (1) and (2). The variations of the perpendicular and parallel dielectric constants with frequency have been given Fig. 9.

The dielectric anisotropy, $\Delta\varepsilon$ has been calculated via perpendicular and parallel dielectric constants by Eq. (3). The frequency dependent dielectric anisotropies have been shown in Fig. 10 for both LCs. According to Fig. 10, the sign of the dielectric anisotropy changes from positive to negative with the different critical frequencies for **5CB** and **5CB+(1%)BAC**. The related critical frequencies have been determined as 433.5 kHz and 439.5 kHz for **5CB** and **5CB+(1%)BAC** composites, respectively. From this point of view, it has been observed that adding **BAC** liquid crystal to **5CB** system increases dielectric anisotropy. Since the larger the dielectric anisotropy, the smaller electric field is needed to reorient the LC molecules, it has been deduced that **BAC** doping makes the orientation of molecules easier.

According to Maier and Meier, it is accepted that the order parameter approximately equals to dielectric anisotropy [27]. From this point of view, it has been revealed that **BAC** doping increases the order in **5CB** liquid crystal system.

The splay elastic constants have also been calculated by Eq. (6) for the related LCs. The Fréedericksz threshold voltages and dielectric anisotropies have been determined by

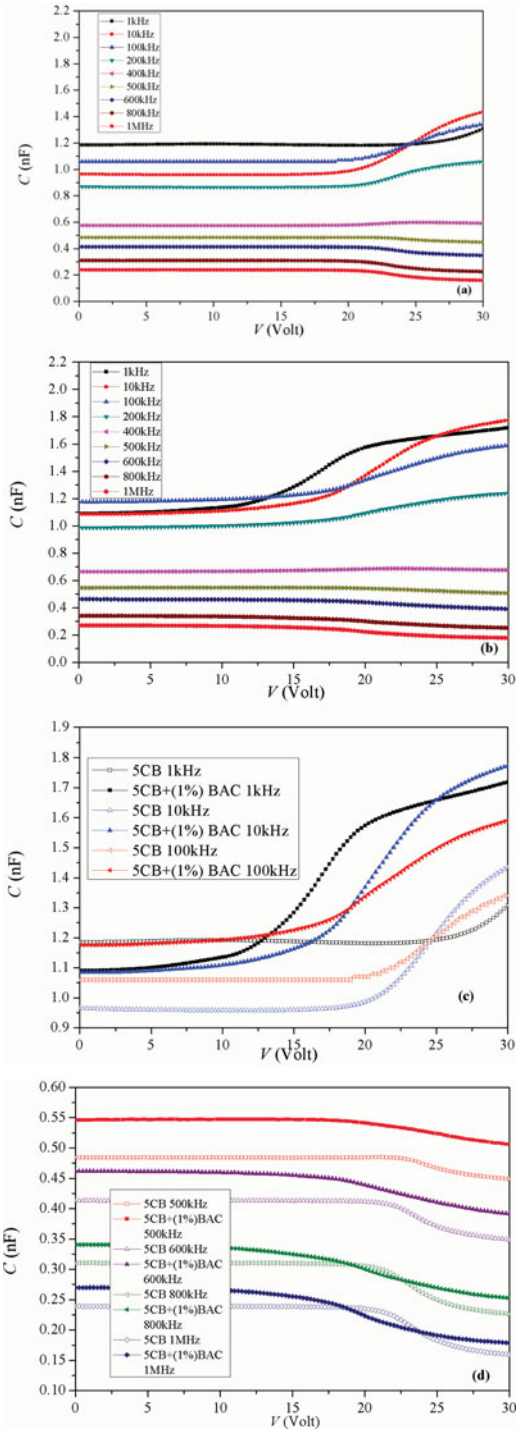


Figure 8. The variation of capacitance with applied voltages for **(a) 5CB** and **(b) 5CB+(1%)BAC** composite. The effect of adding **BAC** liquid crystal to **5CB** system on *C-V* curves for **(c)** 1–100 kHz frequency region **(d)** 500 kHz–1 MHz frequency region.

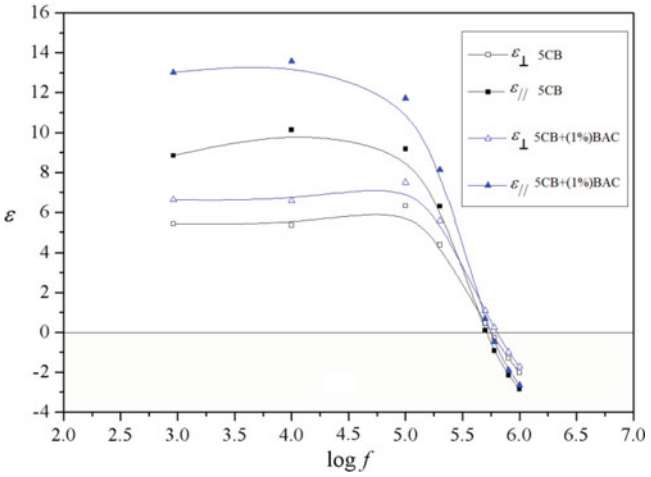


Figure 9. The variations of perpendicular and parallel dielectric constants with frequency for **5CB** and **5CB+(1%)BAC** compounds.

Figs. 8a, 8b, and 10, respectively. The related Fréedericksz threshold voltages and dielectric anisotropies have been listed in Table 1.

The frequency dependent splay constants have been given in Fig. 11 for **5CB** and **5CB+(1%)BAC**.

As is seen from Fig. 11, adding **BAC** liquid crystal to **5CB** decreases the splay elastic constant. In this respect, it has been revealed that doping **BAC** to **5CB** compound decreases distortions in the system.

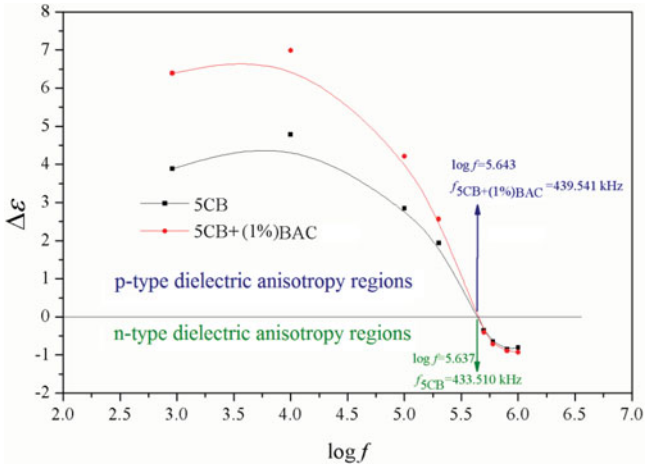


Figure 10. The variations of dielectric anisotropy with frequency of **5CB** and **5CB+(1%)BAC**.

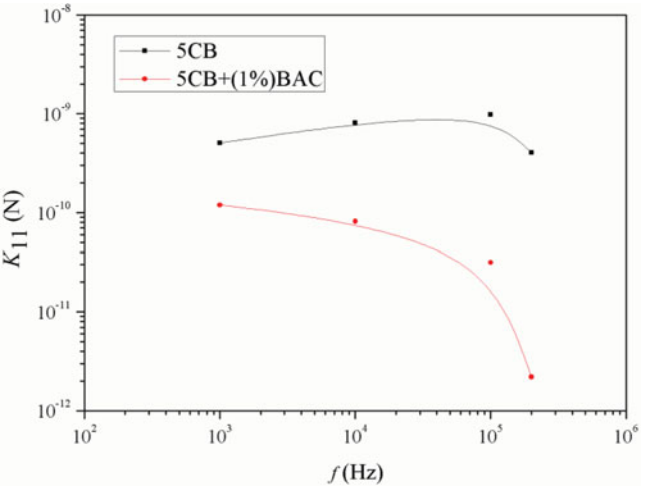


Figure 11. The variations of splay constant, K_{11} with frequency applied for **5CB** and **5CB+(1%)BAC** LCs.

5. Conclusions

In this work, we have reported significant changes in threshold voltage, dielectric anisotropy, critical frequency, and splay elastic constant by adding 1% (w/w) **BAC** to **5CB** liquid crystal. It has been observed that while dielectric anisotropy and critical frequency increase with doping **BAC** to **5CB,** threshold voltage and splay elastic constant decrease. From this point of view, **BAC** doping manifests itself as an increase of the order and decrease of the deformation in **5CB** liquid crystal system. Ultimately, it has been revealed that adding **BAC** to **5CB** makes molecule orientation easier referring to reduction in threshold voltage which has a key role in electro-optic applications.

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