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Liquid Crystals

Publication details, including instructions for authors and subscription information:
<http://www.tandfonline.com/loi/tlct20>

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Published online: 13 Jan 2015.



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To cite this article: D. Venkata Sai, K. P. Zuhail, Rudraditya Sarkar & Surajit Dhara (2015) Structure-property correlation of bicyclohexane nematic liquid crystals, *Liquid Crystals*, 42:3, 328-333, DOI: [10.1080/02678292.2014.987708](https://doi.org/10.1080/02678292.2014.987708)

To link to this article: <http://dx.doi.org/10.1080/02678292.2014.987708>

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Structure–property correlation of bicyclohexane nematic liquid crystals

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(Received 7 October 2014; accepted 11 November 2014)

We report measurements of birefringence, dielectric anisotropy, splay and bend elastic constants of a homologous series of bicyclohexane nematic liquid crystals. These liquid crystals exhibit low birefringence and high negative dielectric anisotropy. In the nematic phase, the ratio of bend to splay elastic constant is less than 1 ($K_{33}/K_{11} \simeq 0.7$). The low birefringence, high negative dielectric anisotropy and low elastic constant ratio are discussed based on the optimised molecular structure obtained from density functional calculations.

Keywords: bicyclohexane nematic liquid crystals; birefringence; elastic constants; density functional theory

1. Introduction

The physical properties of liquid crystals such as optical, dielectric and viscoelastic properties strongly depend on the molecular structure. The electrooptical response of the liquid crystal displays (LCDs) depends on the physical properties. Usually calamitic liquid crystals (made of rod-like molecules) are used for LCD applications. In order to improve the performance of LCDs, efforts have always been made to synthesise new molecules. This led to the discovery of many liquid crystals with new phases and physical properties. A class of such liquid crystals are known as bent-core liquid crystals. The effective shapes of the constituent molecules are bent type. Occasionally the bent-shaped molecules also show nematic phase and mostly they exhibit negative dielectric anisotropy, lower bend elastic constant, large rotational viscosity and flexo-electric coefficients. It has been established that the molecular shape has a significant role on the above mentioned physical properties.[1–7]

Recently, a nematic liquid crystal with bicyclohexane core (CCN-47) has been reported to show a discontinuous anchoring transition with a large thermal hysteresis on perfluoropolymer-treated cells.[8] Subsequently, several physical phenomena and new applications of this transition have been reported. For example, it has been exploited to demonstrate rewritable memory device,[9–11] microflow-induced bistable alignment,[12] and photothermal switching of conductivity in liquid crystal conducting polymer–nanofibre composites.[13] The heat capacity and thermal diffusivity change of discontinuous anchoring transition have also been reported.[14,15] Very recently, the origin of the anchoring transition has

been explained both experimentally and theoretically.[16] The molecular structure of this liquid crystal is very different from conventional liquid crystals made of one or more phenyl rings. These interesting results and optical effects encouraged us to measure the physical properties and understand the structure–property correlation of these bicyclohexane liquid crystals. In this paper, we report on the measurements of some physical properties such as birefringence, dielectric anisotropy, splay and bend elastic constants as a function of temperature. The results are discussed based on the optimised molecular structure obtained from the density functional theory (DFT).

2. Experimental

For measuring physical properties, cells were prepared by two indium tin oxide (ITO)-coated glass plates with circularly patterned electrodes. The plates were spin coated with polyimides (AL-1254 and JALS-204) and cured at 180°C and 200°C, respectively, for 1 h and rubbed antiparallel way for planar and homeotropic alignment of the director (the average alignment direction of the molecules). Cells were made by placing the two plates together, ensuring that the electrode area overlaps. The separation was controlled by glass-bead spacers with diameters 8–13.5 μm for various measurements. The thickness of the empty cell was measured with ±1% accuracy by an interferometric technique using a spectrometer (Ocean Optics, HR-4000). The empty cell was heated and filled with the sample in the isotropic phase. The alignment of the sample was observed using a polarising optical microscope (Nikon, LV100 POL) and a temperature controller

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(Instec, mK 1000). The temperature-dependent birefringence in a planar cell was measured by using a phase modulation technique [17] with the help of a helium–neon laser, photoelastic modulator (PEM-100) and a lock-in amplifier. The dielectric constants are measured by using an LCR meter (Agilent E4980A). The parallel component of the dielectric constant was measured in a homeotropic cell at an applied voltage of 0.2 V below the Freedericksz threshold voltage. To measure the perpendicular component of dielectric constant, the effective dielectric constant was measured as a function of applied voltage (from 0.02 V to 15 V in steps of 0.02 V) at various temperatures. The experimental variation of the voltage-dependent dielectric constant tends to saturate at high voltages. The linear part of the dielectric constant is plotted against $1/V$ and extrapolated to $1/V = 0$ to obtain ϵ_{\perp} at various temperatures. The measured value is in good agreement with the measurement made in planar cells. The bend elastic constant (K_{33}) is obtained from the electric field-induced Freedericksz transition [18] and is given by $K_{33} = \epsilon_0 |\Delta\epsilon| (V_{th}/\pi)^2$, where V_{th} is the Freedericksz threshold voltage and $\Delta\epsilon = (\epsilon_{\parallel} - \epsilon_{\perp})$ is the dielectric anisotropy. K_{11} was estimated from the fitting of the voltage-dependent dielectric constant with the theoretical equations [19]:

$$\frac{V}{V_{th}} = \frac{2}{\pi} \sqrt{1 + \gamma \sin^2(\phi_m)} \times \int_{\psi=0}^{\psi=\frac{\pi}{2}} \sqrt{\frac{1 + \kappa \sin^2(\phi_m) \sin^2(\psi)}{(1 + \gamma \sin^2(\phi_m) \sin^2(\psi))(1 - \sin^2(\phi_m) \sin^2(\psi))}} d\psi \quad (1)$$

$$\epsilon_{eff}(V) = \epsilon_{\parallel} \times \left(\frac{\int_{\psi=0}^{\psi=\frac{\pi}{2}} \sqrt{\frac{(1 + \kappa \sin^2(\phi_m) \sin^2(\psi))(1 + \gamma \sin^2(\phi_m) \sin^2(\psi))}{(1 - \sin^2(\phi_m) \sin^2(\psi))}} d\psi}{\int_{\psi=0}^{\psi=\frac{\pi}{2}} \sqrt{\frac{(1 + \kappa \sin^2(\phi_m) \sin^2(\psi))}{(1 + \gamma \sin^2(\phi_m) \sin^2(\psi))(1 - \sin^2(\phi_m) \sin^2(\psi))}} d\psi} \right) \quad (2)$$

where ϵ_{eff} is the effective dielectric constant, ϕ_m is the tilt angle at the middle of the cell and the other terms of the reduced quantities are $\gamma = (\epsilon_{\perp}/\epsilon_{\parallel}) - 1$, $\kappa = (K_{11}/K_{33}) - 1$. ϕ is the z -dependent tilt angle and ϕ_m is the maximum tilt angle at the middle of the cell ($z = d/2$) and substituted with $\sin(\phi) = \sin(\phi_m)\sin(\psi)$. The dielectric constant at higher voltage are fitted to the above equations by an iterative procedure to get the splay elastic constant K_{11} . [20]

3. Results and discussion

The phase transition temperatures of the compounds 4,4'-dialkyl-(1 α ,1' α -bicyclohexyl)-4 β -carbonitrile (CCN-mn) are shown in Table 1. All the compounds have the same core with varying alkyl chain length on both sides (Figure 2). The compound CCN-35 exhibits only nematic (N) phase. CCN-38 and CCN-47 exhibit nematic and smectic-A (SmA) phases. The remaining compounds CCN-46, CCN-55 and CCN-73 exhibit nematic and smectic-B (SmB) phases. Some physical characterisations such as X-ray, NMR and dielectric relaxation studies on some of these compounds have been reported.[21–27]

The variation of dielectric anisotropy ($\Delta\epsilon$) with shifted temperature is shown in Figure 1. The dielectric anisotropy is negative ($\Delta\epsilon < 0$) in all the compounds and exhibits a typical behaviour, that is, $\Delta\epsilon$ increases with decreasing temperature. At a relative temperature, the dielectric anisotropy is largest for CCN-35 and lowest for CCN-47. The variation of birefringence (Δn) of the compounds with shifted temperature is shown in the inset of Figure 1. The birefringence is very low in all the compounds, for example, near the room temperature $\Delta n \approx 0.03$. It may be mentioned that Δn is more than five times lower than the very well-known liquid crystal, for

Table 1. Phase transition temperatures of the compounds.

Compounds	Phase transition temperatures (°C)
CCN-35	Cr 38.4 N 49.3 I
CCN-38	Cr 41 SmA (23) N 49.5 I
CCN-46	Cr 30 SmB (26) N 54.7 I
CCN-47	Cr 25.6 SmA 28.2 N 57.3 I
CCN-55	Cr 25 SmB 30 N 66.4 I
CCN-73	Cr 38.6 SmB (38) N 50.2 I

Note: Cr, crystal; N, nematic; SmA, smectic-A; SmB, smectic-B.

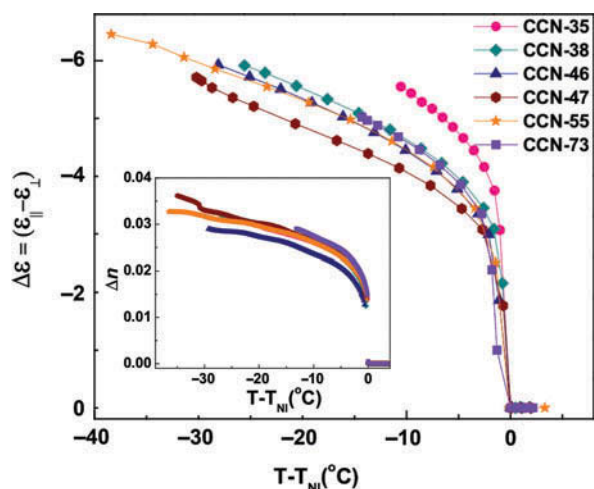


Figure 1. (colour online) Variation of dielectric anisotropy ($\Delta\epsilon$) of the compounds as a function of shifted temperature. Frequency for the dielectric measurement is 4111 Hz. (Inset) Temperature variation of birefringence (Δn) measured at $\lambda = 632.8$ nm.

example, 5CB (pentyl cyanobiphenyl). The birefringence of bicyclohexane compounds with longitudinal cyano group such as nCCH (trans, trans-4'-*n*-alkylbicyclohexyl-4-carbonitriles) has been reported by several authors.[28] It appears that the birefringence of CCN-*mn* homologues is somewhat lower (about 25%) than that of nCCH compounds.

In order to understand the structure–property correlation, we performed ground state electronic structure calculations of all the molecules with the help of the DFT by using GAUSSIAN-09 suite programming package. All the calculations are performed in the gas phase and optimisation of the structures is done by B3LYP level of theory using cc-pVDZ basis set.[29] Figure 2 shows the two-dimensional (2D) projection of optimised structures of the molecules. It is observed that the molecules are not linear and their 2D projections (keeping the cyano group along the *y*-axis and bicyclohexane along the *x*-axis) are bent-shaped. The principal components of the dipole moments and

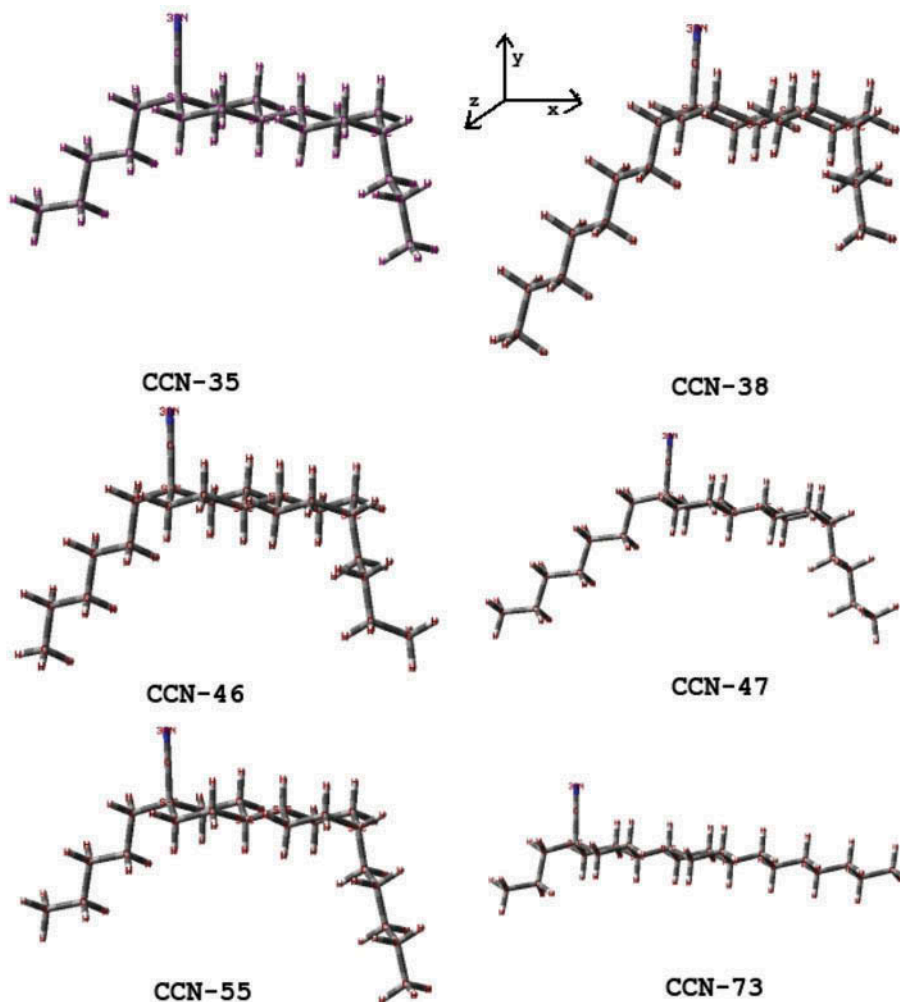


Figure 2. (colour online) Two-dimensional projection of the energy-minimised molecular structures obtained by DFT calculations in the gas phase.

Table 2. Components of dipole moment and principal polarisabilities obtained from DFT calculations.

Compounds	Dipole moment (D)			Polarisability (a.u.)		
	μ_x	μ_y	μ_z	α_{xx}	α_{yy}	α_{zz}
CCN-35	0.276	3.818	0.438	262.56	225.34	216.53
CCN-38	0.726	3.757	0.314	308.70	259.53	244.50
CCN-46	0.138	3.864	0.159	286.48	248.99	239.52
CCN-47	0.165	3.903	0.186	304.48	257.39	249.64
CCN-55	0.910	3.639	0.932	283.67	256.86	235.70
CCN-73	0.482	2.199	3.158	295.61	224.72	262.47

polarisabilities are listed in Table 2. The transverse components of dipole moments (μ_y or μ_z) are much larger in magnitude than that of the longitudinal components (μ_x). For example, in CCN-35, $\mu_x = 0.276$ D, $\mu_y = 3.818$ D and $\mu_z = 0.438$ D, respectively. This explains the origin of large negative dielectric anisotropy in all the compounds. The polarisabilities of all the compounds are larger along the long molecular axis (x -axis) compared to the components in the y and z directions. The birefringence of the compounds is proportional to the polarisability anisotropy ($\Delta\alpha$). In uniform sample, the polarisability anisotropy can be defined as $\Delta\alpha \approx \alpha_{xx} - (\alpha_{yy} + \alpha_{zz})/2$. The average $\Delta\alpha$ of all the compounds is about 50 (a.u.) and it is about five times lower than that of 5CB [30] and consistent with five times lower birefringence of CCN-mn compounds.

The splay and bend elastic constants (K_{11} and K_{33}) were measured from the voltage-dependent dielectric constant data in the homeotropic cell as described in the experimental section. The variation of splay (K_{11}) and bend (K_{33}) elastic constants as a function of temperature is shown in Figure 3. The variation of ϵ_{eff} together with the best fit of Equations (1) and (2) is also shown in the inset of Figure 3(a). Both K_{11} and K_{33} of all the compounds (except CCN-47) in the nematic phase increase with decreasing temperature. In addition, both the elastic constants show presmectic divergence in CCN-47 compound. The ratio of K_{33}/K_{11} is shown in the inset of Figure 3(b). Interestingly, it is observed that K_{33} is lower than K_{11} , that is, $K_{33}/K_{11} \simeq 0.7$, except very close to the SmA phase transition temperature of CCN-47. Similar behaviour may also be expected in CCN-38 but the N-SmA transition temperature is below the ambient and beyond accessible temperature range of our temperature controller. The presmectic divergence of K_{11} is rare as the splay distortion is permitted even in the smectic-A phase. However, there are a few reports showing presmectic divergence of both K_{11} and K_{33} . [2,20] In case of bent-core nematic liquid crystals, it has been reported that $K_{33} < K_{11}$ and occasionally they exhibit unusual temperature

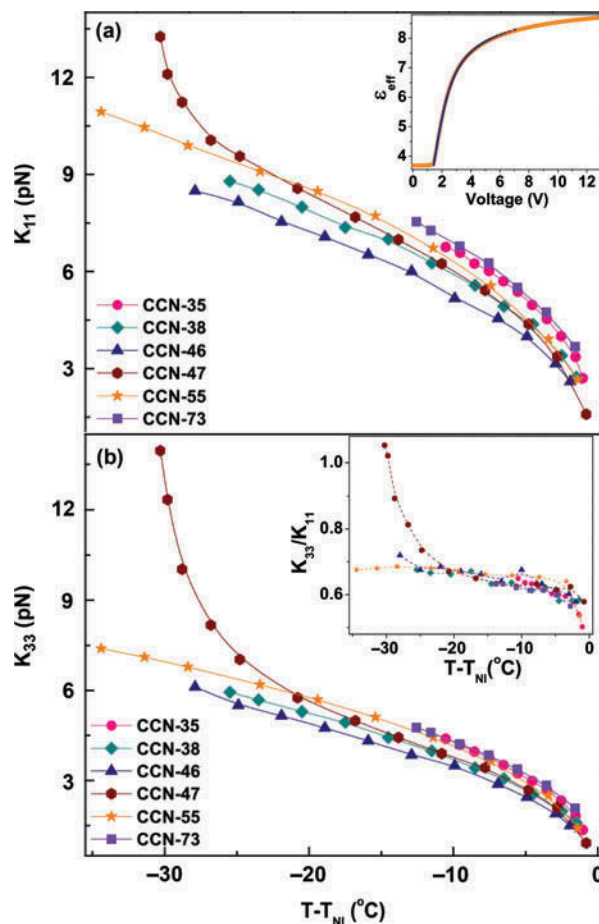


Figure 3. (colour online) (a) Variation of splay elastic constant (K_{11}) as a function of shifted temperature. (Inset) Effective dielectric constant as a function of applied voltage. Solid black line is a theoretical fit to the experimental data. (b) Temperature variation of bend elastic constant (K_{33}). (Inset) Temperature variation of the ratio, K_{33}/K_{11} .

dependence.[1,4] It was suggested that the strain in the bend distortion is partly relieved if the molecules are curved or bent shaped and consequently K_{33} is expected to be lower than K_{11} . [31] The energy-minimised structures of the present calamitic molecules are bent type (Figure 2) and expected to be

responsible for the similar results as that of bent-core nematic liquid crystals.

It may be useful to discuss and compare the elastic constant ratio with bicyclohexane nematic compounds such as nCCH.[32] It was reported that the elastic constant ratio of nCCH is always greater than 1 (i.e. $K_{33}/K_{11} > 1$). This is in contrast to the observed effect in the present compounds. The important structural difference between the two homologous series of nCCH and CCN-mn is the position of the cyano group (-CN). In case of nCCH, the cyano group is at the longitudinal position, whereas in CCN-mn, it is in the lateral position. In addition, the alkyl chains are present on both sides of bicyclohexane. The side chains of CCN-mn increase the flexibility of the molecules. Apart from the enhanced flexibility, the transverse dipole moment of CCN-mn molecules can have a significant role on the ratio of the curvature elastic constants. It was proposed that the effect of dipole moment on the elastic constants is connected to the local ordering of the dipoles in nCCH compounds.[33] The effective molecular length could be greater in nCCH compounds because of the antiparallel local ordering of the molecules with the overlapped cyano group. It has been shown both experimentally and theoretically that in nematic liquid crystals, $K_{33}/K_{11} \propto (L/W)^2$, where L is the length and W is the width of the mesogenic molecule, respectively.[31] Thus, the lower ratio of K_{33}/K_{11} of CCN-mn compounds than nCCH compounds partially could be due to the absence of local ordering, apart from the effect of molecular shape.

4. Conclusion

In conclusion, we have measured the birefringence, dielectric anisotropy, splay and bend elastic constants of homologous series of bicyclohexane nematic liquid crystals as a function of temperature. The optimised molecular structure obtained from the calculation of DFT shows that the molecules are bent-shaped with large transverse dipole moments and low polarisability anisotropy. The low birefringence, high negative dielectric anisotropy and low elastic constant ratio of the compounds are explained based on the optimised molecular properties.

Acknowledgements

We gratefully acknowledge support from the DST (SR/NM/NS-134/2010) and CSIR (03(1207)/12/EMR-II), DST PURSE and UPE-II. VD acknowledges UGC for fellowship. We thank Prof. W. Haase for providing CCN-mn compounds. RS acknowledges UGC for doctoral

fellowship. We thank Prof. S. Mahapatra, School of Chemistry, UoH, for useful discussion.

References

- [1] Sathyanarayana P, Mathews M, Li Q, Sastry VSS, Kundu B, Le KV, Takezoe H, Dhara S. Splay bend elasticity of a bent-core nematic liquid crystal. *Phys Rev E*. 2010;81:010702R-1–010702R-4. DOI:10.1103/PhysRevE.81.010702.
- [2] Sathyanarayana P, Varia MC, Prajapati AK, Kundu B, Sastry VSS, Dhara S. Splay-bend elasticity of a nematic liquid crystal with T-shaped molecules. *Phys Rev E*. 2010;82:050701R-1–050701R-4. DOI:10.1103/PhysRevE.82.050701.
- [3] Arun Kumar T, Le KV, Kim JK, Takezoe H, Dhara S. Alignment of unconventional nematic liquid crystals. *Liq Cryst*. 2011;38:917–924. DOI:10.1080/02678292.2011.585522.
- [4] Sathyanarayana P, Radhika S, Sadashiva BK, Dhara S. Structure-property correlation of a hockey stick-shaped compound exhibiting N-SmA-SmC_a phase transitions. *Soft Matter*. 2012;8:2322–2327. DOI:10.1039/c2sm06767f.
- [5] Kaur S, Tian L, Liu H, Greco C, Ferrarini A, Seltmann J, Lehmann M, Gleeson HF. The elastic and optical properties of a bent-core thiadiazole nematic liquid crystal: the role of the bend angle. *J Mater Chem C*. 2013;1:2416–2425. DOI:10.1039/c3tc00852e.
- [6] Kaur S, Addis J, Greco C, Ferrarini A, Görtz V, Goody JW, Gleeson HF. Understanding the distinctive elastic constants in an oxadiazole bent-core nematic liquid crystal. *Phys Rev E*. 2012;86:041703-1–041703-11. DOI:10.1103/PhysRevE.86.041703.
- [7] Jákli A. Liquid crystals of the twenty-first century – nematic phase of bent-core molecules. *Liq Cryst Rev*. 2013;1:65–82. DOI:10.1080/21680396.2013.803701.
- [8] Dhara S, Kim JK, Jeong SM, Kogo R, Araoka F, Ishikawa K, Takezoe H. Anchoring transitions of transversely polar liquid-crystal molecules on perfluoropolymer surfaces. *Phys Rev E*. 2009;79:060701R-1–060701R-4. DOI:10.1103/PhysRevE.79.060701.
- [9] Kim JK, Araoka F, Jeong SM, Dhara S, Ishikawa K, Takezoe H. Bistable device using anchoring transition of nematic liquid crystals. *Appl Phys Lett*. 2009;95:063505-1–063505-3. DOI:10.1063/1.3202781.
- [10] Kim JK, Le KV, Dhara S, Araoka F, Ishikawa K, Takezoe H. Heat-driven and electric-field-driven bistable devices using dye-doped nematic liquid crystals. *J Appl Phys*. 2010;107:123108-1–123108-4. DOI:10.1063/1.3446826.
- [11] Kumar TA, Le KV, Aya S, Kang S, Araoka F, Ishikawa K, Dhara S, Takezoe H. Anchoring transition in a nematic liquid crystal doped with chiral agents. *Phase Trans*. 2012;85:888–899. DOI:10.1080/01411594.2012.692092.
- [12] Jampani VSR, Skarabot M, Takezoe H, Mušević I, Dhara S. Laser-driven microflow-induced bistable orientation of a nematic liquid crystal in perfluoropolymer-treated unrubbed cells. *Opt Express*. 2013;21:724–729. DOI:10.1364/OE.21.000724.
- [13] Rasna MV, Zuhail KP, Manda R, Paik P, Haase W, Dhara S. Discontinuous anchoring transition and photo-thermal switching in composites of liquid

- crystals and conducting polymer nanofibers. *Phys Rev E*. 2014;89:052503-1–052503-5. DOI:10.1103/PhysRevE.89.052503.
- [14] Aya S, Sasaki Y, Pocięcha D, Araoka F, Górecka E, Ema K, Mušević I, Orihara H, Ishikawa K, Takezoe H. Stepwise heat-capacity change at an orientation transition in liquid crystals. *Phys Rev E*. 2014;89:022512-1–022512-5. DOI:10.1103/PhysRevE.89.022512.
- [15] Uehara M, Aya S, Araoka F, Ishikawa K, Takezoe H, Morikawa J. Discontinuous thermal diffusivity change due to the anchoring transition of a liquid crystal on a perfluoropolymer surface. *J Chem Phys Chem*. 2014;15:1452–1456.
- [16] Sai DV, Kumar TA, Haase W, Roy A, Dhara S. Effect of smectic short-range order on the discontinuous anchoring transition in nematic liquid crystals. *J Chem Phys*. 2014;141:044706-1–044706-6. DOI:10.1063/1.4890532.
- [17] Oakberg TC. Measurement of low-level strain birefringence in optical elements using a photoelastic modulator. *Proc SPIE*. 1996;2873:17–20. DOI:10.1117/12.246208.
- [18] Freedericksz V, Zolina V. Forces causing the orientation of an anisotropic liquid. *Trans Faraday Soc*. 1933;29:919. DOI:10.1039/tf9332900919.
- [19] Gruler H, Scheffer TJ, Meier G. Elastic constants of nematic liquid crystals. *Z Naturforsch*. 1972;27A:966.
- [20] Morris SW, Palfy P, Balzarini DA. Measurements of the bend and splay elastic constants of octyl-cyanobiphenyl. *Mol Cryst Liq Cryst*. 1986;139:263–280. DOI:10.1080/00268948608080132.
- [21] Walz L, Haase W, Eidenschink R. The crystal and molecular structures of four homologous, mesogenic trans,trans-4,4'-dialkyl-(1 α ,1'-bicyclohexyl)-4 β -carbonitril (CCN's). *Mol Cryst Liq Cryst*. 1989;168:169–182.
- [22] Eidenschink R, Haas G, Römer M, Scheuble BS. Liquid-crystalline 4-bicyclohexylcarbonitriles with extraordinary physical properties. *Angew Chem*. 1984;23:147. DOI:10.1002/anie.198401471.
- [23] Ganzke D, Wróbel S, Haase W. Dielectric studies of bicyclohexylcarbonitrile nematogens with large negative dielectric anisotropy. *Mol Cryst Liq Cryst*. 2004;409:323–333. DOI:10.1080/1542140_0490431660.
- [24] Dhara S, Madhusudana NV. Physical characterisation of 4'-butyl-4-heptyl-bicyclohexyl-4-carbonitrile. *Phase Trans*. 2008;81:561–569. DOI:10.1080/01411590801975401.
- [25] Dhara S, Madhusudana NV. Enhancement of the orientational order parameter of nematic liquid crystals in thin cells. *Euro Phys J E*. 2004;13:401–408. DOI:10.1140/epje/i2003-10084-8.
- [26] Dhara S, Madhusudana NV. Influence of director fluctuations on the electric-field phase diagrams of nematic liquid crystals. *Euro Phys Lett*. 2004;67:411–417. DOI:10.1209/epl/i2004-10078-8.
- [27] Zawadzki A, Walton HG. Measurements of the splay and bend elastic constants of 4'-butyl-4-heptyl-bicyclohexyl-4-carbonitrile, CCN47. *Mol Cryst Liq Cryst*. 2012;569:10–14. DOI:10.1080/15421406.2012.691070.
- [28] Ibrahim IH, Haase W. On the molecular polarizability of nematic liquid crystals. *Mol Cryst Liq Cryst*. 1981;66:189–198. DOI:10.1080/00268948108072672.
- [29] Dunning TH. Gaussian basis sets for use in correlated molecular calculations. I. The atoms boron through neon and hydrogen. *J Chem Phys*. 1989;90:1007–1023. DOI:10.1063/1.456153.
- [30] Demus D, Inukai T. Calculation of molecular, dielectric and optical properties of 4'-n-pentyl-4-cyano-biphenyl (5CB). *Liq Cryst*. 1999;26:1257–1266. DOI:10.1080/026782999203922.
- [31] De Jeu WH. Physical properties of liquid crystalline materials. London: Gordon and Breach; 1980.
- [32] Bradshaw MJ, Raynes EP. Electric permittivities and elastic constants of the cyano bi-cyclohexanes (CCH). *Mol Cryst Liq Cryst*. 1981;72:35–42. DOI:10.1080/01406568108084034.
- [33] Brownsey GJ, Leadbetter AJ. Novel liquid crystal structures in cyano bi-cyclohexanes. *J Physique Lett*. 1981;42:135–140. DOI:10.1051/jphyslet:01981004206013500.