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Synthesis of New Nondisk-Shaped Thermotropic Liquid Crystalline Compounds Showing a Rectangular Columnar Mesophase

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Linear- and polycatenar-type compounds possessing a cabazole moiety as a head group, linked to the trialkoxy terminal tails via a linear aromatic chain have been designed and synthesized. These compounds exhibit a liquid crystalline rectangular columnar phase. The mesomorphic nature was determined by polarizing optical microscopy (POM) and differential scanning calorimetry (DSC) in combination with powder XRD.

Keywords Carbazole; differential scanning calorimetry; polarizing optical microscopy; rectangular columnar phase; Schiff's base; X-ray diffraction

Introduction

During the last decades, columnar liquid crystalline materials have received greater interest due to the their enormous applications such as organic semiconductors [1,2], photovoltaic cells, optical light-emitting diodes [3,4], etc. Columnar hexagonal (Col_h) and columnar rectangular (Col_r) phases are the most common in case of discotic molecules. However, certain molecules that are not disk-shaped may also exhibit such columnar mesophases depending on their supramolecular arrangements [5–8]. They may be bow-like [9] or polycatenars [10,11], i.e., the compound consists of a rod-like or bent mesogenic core with multiple terminal alkyl chains. The shape of the molecule, that is, symmetry in structure, dipole–dipole interaction, and π-stacking interactions are the key elements in forming the supramolecular arrangements of the molecules [12]. The polar order in columnar phases is quite rare [13] as in most cases the molecules are highly symmetrical. It was found in either bow-like or chiral disk-like molecules. A columnar superstructure can be generated in the mesophases by using intermolecular attractive interactions, such as dipole–dipole and arene-perfluoroarene. In the superstructures, arene-perfluoroarene face-to-face interactions should be the main attractive forces for the molecular stacking. Several interactions, such as hydrogen bonding, dipole–dipole interactions, ionic bonding, charge-transfer complexation, and microsegregation, were used recently for the generation of superstructures in liquid crystal phases [14–20].

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In addition to their extensive biological activity, carbazole derivatives have vast application in material science such as photorefractive materials, optical data storage, optical image processing, electroluminescence, nonlinear optics, and photoconductivity [21]. The tendency of N-alkyl carbazole derivatives to self-assemble a three-dimensional network via π-π stacking, electrostatic forces, and van der Waals interactions forming an organogel is very high [22]. Various types of disk-shaped or symmetrical rod or bent-shaped polycatenar-type mesogens are known to self-organize into a columnar phase [23–27]. However, only a few examples of such nondisk-shaped unsymmetrical linear-type mesogens assembled into a columnar phase [7,8] are reported so far. Considering all the aforesaid aspects and in continuation of our interest in the design and synthesis of new chiral [28–31] and achiral [32–34] liquid crystalline materials, we have designed a series of compounds consisting of N-methyl carbazole as the head group and trialkoxy terminal chains linked via mesogenic aromatic chain. In the molecules there are three basic units that are responsible for the interaction between the molecular segments forming the mesophase, viz., terminal alkoxy tails, aromatic unit consisting of imine and ester linkages, and the rigid central heteroaromatic head group. Therefore, we have undertaken a study to synthesize the aforesaid compounds and study their mesomorphic properties. Here, we report the results of our investigation.

Results and Discussion

The requisite amine precursor (**1**) and the aldehyde precursors (**2a-d**) were synthesized following the published procedures [35,36].

The target compounds **3a–d** were synthesized by the Schiff's base formation of amine **1** with stoichiometric amounts of aldehydes **2a–d** (Fig. 1) in refluxing ethanol in the presence of a catalytic amount of glacial acetic acid for 5 hr (Scheme 1). The compounds **3a–d** were purified by repeated washing with hot ethanol. These were characterized from their elemental analyses and spectral data.

Mesomorphism

The mesomorphic behavior of compounds **3a-d** was initially studied by polarizing optical microscopy (POM). In the POM study, when the compound **3a** was allowed to cool very slowly from the isotropic melt state, the optically birefringent domains slowly grow in a dark background at about 80°C (Fig. 2(a)). The phase was randomly oriented with a planar domain. Compound **3b** was found to be nonmesogenic showing a direct transition from

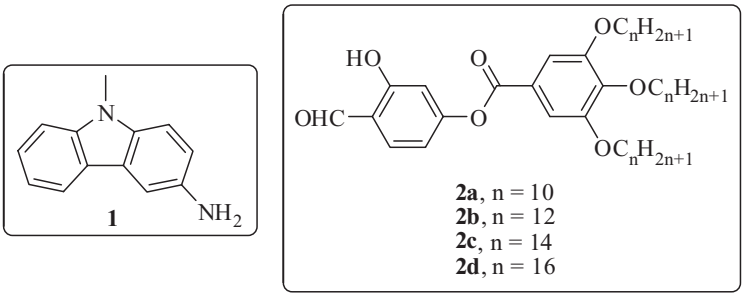
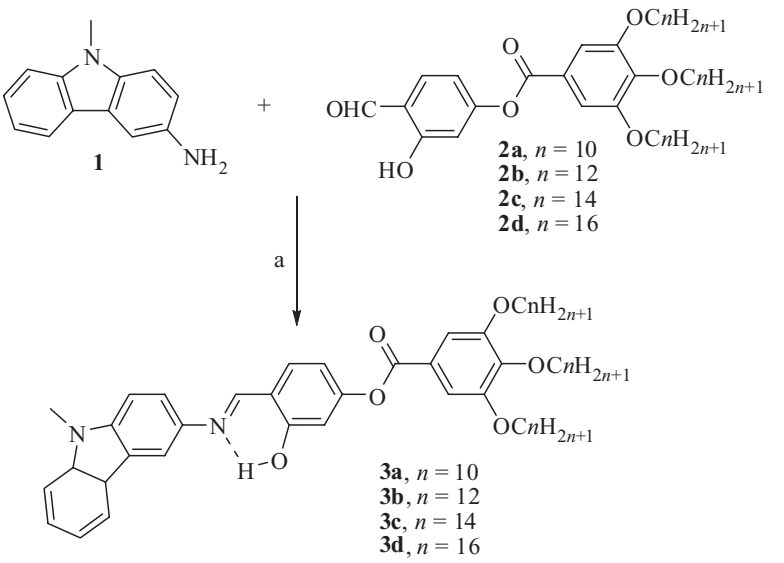


Figure 1. Chemical structures of the precursors.



Scheme 1. Reagents and conditions: (a) absolute EtOH, glacial AcOH, reflux, 5 hr.

the crystalline to the isotropic liquid state at about 75°C in the heating cycle. In case of compound **3c**, a similar type of ribbon-like texture was observed at about 68°C (Fig. 1(b)) in the cooling cycle. Compound **3d** also displayed the same textural appearance at about 63°C during cooling. For all the compounds **3a**, **3c**, and **3d** in the heating cycle, the same mesophases appeared as in case of the cooling cycle. This type of ribbon-like texture is characteristic of a columnar arrangement. The generation of such ribbon-like textures suggests that the growth of the column in the direction of the column axis is much faster than that in the perpendicular direction to the column axis [37].

Differential scanning calorimetry (DSC) was used to determine the transition temperatures and associated enthalpy changes and these are presented in Table 1. In the DSC analysis, it is found that compound **3b** is not mesomorphic and rest of the compounds show

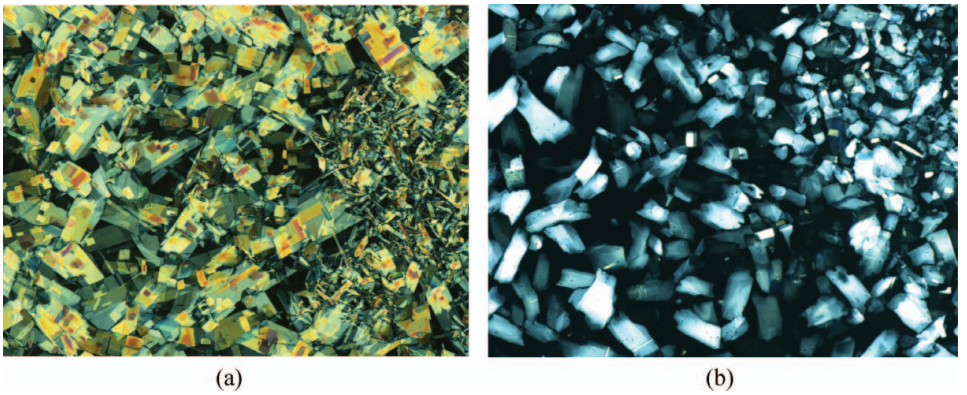


Figure 2. Polarizing optical micrographs: (a) compound **3a** at 80°C and (b) compound **3c** at 68°C.

Table 1. The transition temperatures (°C) and associated enthalpies (in parentheses; kJ mol^{-1}) of the compounds determined by DSC in the second heating and first cooling. Cr, crystal; Col_r, rectangular columnar; I, isotropic liquid

3a	Cr	77.5 (19.7)	→	Col_r	82.1 (1.3)	→	I	48.4 (-22.2) → Cr
3b	Cr	75.4 (38.8)	→	I	51.0 (37.8)	→	Cr	
3c	Cr	61.5 (32.7)	→	Col_r	71.1 (14.8)	→	I	36.5 (-2.2) → Cr
3d	Cr	46.7 (62.3)	→	Col_r	68.2 (17.9)	→	I	36.9 (-56.1) → Cr

Cr = crystal; Col_r = rectangular columnar; I = isotropic liquid

monotropic mesophase transitions [7]. It is also observed that the melting temperature decreases from **3a** to **3d**, i.e., with the increase of the chain length.

Variable temperature powder X-ray scattering experiments were used to confirm the structure of the columnar phase. For compound **3a**, at all the temperatures 58°C, 79°C in the heating cycle, and 45°C in the cooling cycle, a diffuse wide-angle peak is present at about 4.3 Å indicating a liquid-like in-plane order. Taking 79°C into account as the mesophase appears clearly at this temperature, in the small angle region, three sharp reflections are observed at $d_1 = 36.8$ Å, $d_2 = 26.0$ Å, and $d_3 = 17.3$ Å (Fig. 3) associated with

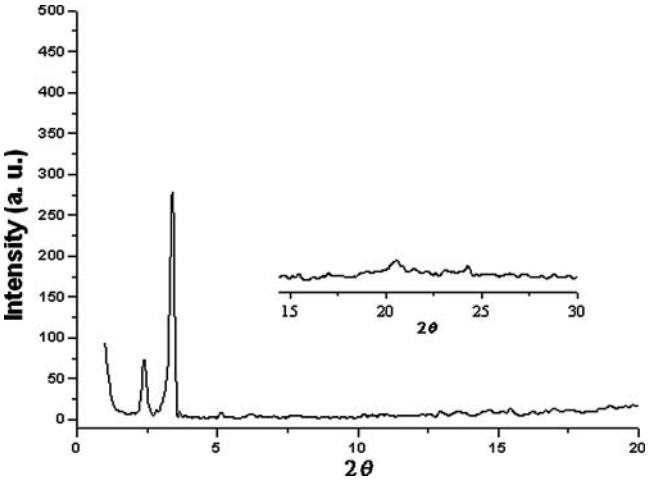


Figure 3. Powder X-ray diffraction pattern of compound **3a** at 79°C.

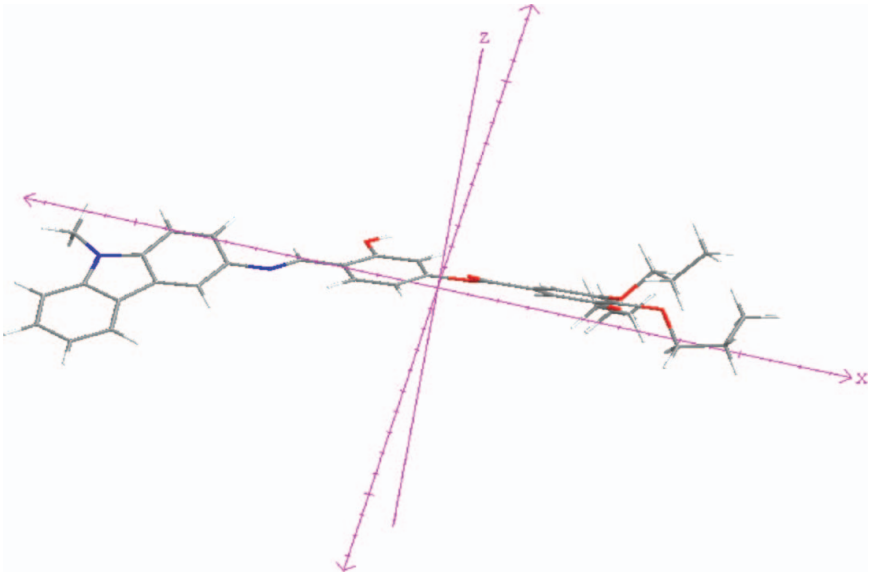


Figure 4. Energy-minimized structure of **3a** (considering up to three-carbon chain length for simplicity).

the (20), (11,11$^-$), and (31,31$^-$) reflections and are indeed characteristic of a rectangular lattice [38]. The lattice parameters of the rectangular cell are $a = 73.56$ Å and $b = 27.74$ Å. Additionally, a sharp peak at 3.7 Å is also present, suggesting the stacking distance of the columns.

The density functional theory (DFT) calculation was carried out on compound **3a** (considering up to three carbon terminal chain length) to determine the nature of dipolar interaction within the molecules. We have computed the DFT (B3LYP) level of theory using the basis set 6-31G to obtain the dipole moment and dipolar orientation of molecules. The dipole moment of **3a** had been calculated as 6.6454 D ($X = -1.5133$, $Y = 6.4102$, $Z = -0.8836$). The geometrically optimized structure of compound **3a** (Fig. 4) suggests that the molecule is nondisk shaped. The first optimization was carried out by the MM2 method followed by the AM1 method, and finally, DFT was performed as stated earlier. The maxima of dipole moment are in the positive y-axis direction (6.4102 D), and the direction of net dipole moment should be transverse to the molecular axis. It can be assumed that the association of the two molecules in an antiparallel fashion generates a full disk shape to cancel out their dipoles forming a pseudoplanar sheet-like arrangement perpendicular to the column axis and the sheets stack up above one another forming the columnar arrangement.

In conclusion, a series of nondisk-shaped molecules based on carbazole with terminal trialkoxy chains of different chain lengths was synthesized. All of the compounds showed mesomorphic behavior. The mesophase was identified by POM, DSC, and X-ray scattering experiments as rectangular columnar. A DFT calculation was also carried out to find out the dipolar interaction between the molecules. From the orientation of the dipole moment, one can conclude that the stacking in the rectangular columnar phase may arise due to the association of the two molecules in an antiparallel fashion generating a full disk shape to cancel out their individual dipoles and form the columnar mesophase [8].

Experimental

General

All of the chemicals were purchased from either Sigma Aldrich Chemicals Pvt. Ltd. or Spectrochem, Mumbai, India. Silica gel (60–120 mesh) was used for chromatographic separation. Silica gel G (Spectrochem) was used for thin layer chromatography. Infrared (IR) spectra were recorded on a Perkin-Elmer L 120-000A spectrometer (ν_{max} in cm^{-1}) on KBr disks. ^1H NMR (500 MHz) and ^{13}C NMR (100 MHz) spectra were recorded on a Bruker DPX-500 spectrometer in $CDCl_3$ (chemical shift in δ) with tetramethylsilane as internal standard. The liquid crystalline properties were established by thermal microscopy (Nikon polarizing microscope LV100POL attached with Instec hot and cold stage HCS302, with STC200 temperature controller configured for HCS302) and the phase transitions were confirmed by DSC (Perkin-Elmer Diamond DSC Pyris1 system). Elemental analysis (C, H, and N) was recorded on a Perkin Elmer 2400 series II CHN analyzer. Powder X-ray diffraction pattern of the sample was obtained on a D8 Advance Bruker AXS diffractometer (operated at 40 kV voltage and 40 mA current and calibrated with standard silicon sample) attached with a temperature controller using Cu Kα ($\lambda = 0.15406$ nm) radiation at the Indian Association for the Cultivation of Science, Jadavpur, Kolkata. All computational calculations have been performed by the Chem3D (version 10) [39] with Gaussian 03 Interface [40].

General Procedure for the Synthesis of Compounds 3a–d

A mixture of 3-amino-9-methyl-9*H*-carbazole **1** (0.05 g, 0.255 mmol) and 4-formyl-3-hydroxyphenyl-3,4,5-tris(dodecyloxy) benzoate **2a** (0.181 g, 0.255 mmol) was refluxed in absolute ethanol (10 mL) in the presence of a catalytic amount (one drop) of glacial acetic acid for 5 hr. The Schiff's base **3a** was precipitated out from the reaction mixture. It was collected by decantation, washed repeatedly with hot ethanol, and dried in vacuum. The other derivatives **3b-d** were also similarly prepared.

Compound 3a: Yield 73%, greenish-yellow solid. IR (KBr): $\upsilon = 3430$, 1726, 1594 cm^{-1}. ^1H NMR ($CDCl_3$, 400 MH_z): δ (ppm) 14.12 (s, 1H, O**H**), 8.74 (s, 1H, C**H**=N), 8.10 (d, $J = 7.6$ Hz, 1H, Ar**H**), 8.02 (s, 1H, Ar**H**), 7.57–7.37 (m, 7H, Ar**H**), 7.24 (m, 1H, Ar**H**), 6.89 (s, 1H, Ar**H**), 6.82 (m, 2H, Ar**H**), 4.05 (m, 6H, OC**H$_2$**), 3.83 (s, 3H, N-C**H$_3$**), 1.87–0.86 (m, 57H, aliphatic hydrogens are overlapped). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 164.6, 162.5, 158.9, 154.3, 153.0, 143.1, 141.7, 140.2, 139.8, 132.7, 126.3, 123.7, 123.4, 122.7, 120.5, 119.7, 119.3, 117.7, 112.6, 110.6, 109.0, 108.8, 108.6, 73.6, 69.3, 32.0, 30.4, 29.7, 29.6, 29.4, 29.2, 26.1, 22.7, 14.1. Anal. Calcd. for $C_{57}H_{80}N_2O_6$: C, 76.99; H, 9.07; N, 3.15%. Found: C, 77.13; H, 8.93; N, 3.11%.

Compound 3b: Yield 78%, greenish-yellow solid. IR (KBr): $\upsilon = 3437$, 1734, 1611 cm^{-1}. ^1H NMR ($CDCl_3$, 500 MHz): δ (ppm) 14.09 (s, 1H, O**H**), 8.81 (s, 1H, C**H**=N), 8.12 (d, $J = 7.7$ Hz, 1H, Ar**H**), 8.06 (d, $J = 2.0$ Hz, 1H, Ar**H**), 7.51 (m, 2H, Ar**H**), 7.47 (d, $J = 8.5$ Hz, 1H, Ar**H**), 7.43 (m, 1H, Ar**H**), 7.41 (s, 2H, Ar**H**), 7.38 (d, $J = 5.1$ Hz, 1H, Ar**H**), 7.27 (s, 1H, Ar**H**), 6.89 (m, 1H, Ar**H**), 6.82 (dd, $J = 8.4$, 2.3 Hz, 1H, Ar**H**), 4.06 (m, 6H, OC**H$_2$**), 3.88 (s, 3H, N-C**H$_3$**), 0.86–1.36 (m, 69H, aliphatic hydrogens are overlapped). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C 164.9, 162.9, 159.2, 154.6, 153.5, 143.5, 142.0, 135.3, 133.0, 126.6, 124.0, 123.8, 123.1, 120.9, 120.1, 119.6, 118.0, 109.4, 109.2, 109.1, 109.0, 74.0, 69.7, 32.4, 30.8, 30.2, 30.1, 30.0, 29.8, 29.7, 29.6, 26.5, 23.1, 14.5 MS (MALDI-TOF);

m/z = 973.7335 [M^++1]. Calculated 973.6955, anal. calcd. for $C_{63}H_{92}N_2O_6$: C, 77.73; H, 9.53; N, 2.88%. Found: C, 77.91; H, 9.69; N, 2.69%.

Compound 3c: Yield 77%, greenish-yellow solid. IR (KBr): υ = 3437, 1734, 1588 cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ (ppm) 14.11 (s, 1H, O**H**), 8.81 (s, 1H, C**H**=N), 8.13 (d, J = 7.6 Hz, 1H, Ar**H**), 8.07 (d, J = 2.0 Hz, 1H, Ar**H**), 7.54–7.43 (m, 4H, Ar**H**), 7.41 (s, 2H, Ar**H**), 7.27 (m, 1H, Ar**H**), 6.90 (d, J = 2.0 Hz, 1H, Ar**H**), 6.81 (dd, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H, Ar**H**), 4.06 (m, 6H, OC**H$_2$**), 3.87 (s, 3H, N–C**H$_3$**), 1.87–0.86 (m, 81H, aliphatic hydrogens are overlapped). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 164.6, 162.6, 158.9, 154.3, 153.0, 143.1, 141.7, 140.2, 139.9, 132.7, 126.3, 123.7, 123.4, 122.7, 120.5, 119.8, 119.3, 117.7, 112.8, 110.6, 109.0, 108.8, 108.6, 73.6, 69.3, 32.0, 30.4, 29.8, 29.7, 29.6, 29.4, 29.3, 29.2, 26.1, 22.7, 14.1. Anal. Calcd. for $C_{69}H_{104}N_2O_6$: C, 78.36; H, 9.91; N, 2.65%. Found: C, 78.34; H, 10.09; N, 2.77%.

Compound 3d: Yield 73%, greenish-yellow solid. IR (KBr): υ = 3402, 1734, 1588 cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ (ppm) 14.11 (s, 1H, O**H**), 8.80 (s, 1H, C**H**=N), 8.12 (d, J = 7.6 Hz, 1H, Ar**H**), 8.07 (d, J = 2.0 Hz, 1H, Ar**H**), 7.53–7.44 (m, 4H, Ar**H**), 7.41 (s, 2H, Ar**H**), 7.27 (m, 1H, Ar**H**), 6.89 (d, J = 2.0 Hz, 1H, Ar**H**), 6.82 (dd, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H, Ar**H**), 4.05 (m, 6H, OC**H$_2$**), 3.89 (s, 3H, N–C**H$_3$**), 1.87–0.86 (m, 93H, aliphatic hydrogens are overlapped). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 164.6, 162.5, 159.0, 154.3, 153.0, 143.1, 141.7, 140.2, 139.9, 132.7, 126.3, 123.7, 123.5, 122.7, 120.5, 119.8, 119.3, 117.7, 112.9, 112.6, 110.6, 109.0, 108.8, 108.6, 73.6, 69.3, 31.9, 30.3, 29.8, 29.7, 29.6, 29.4, 29.3, 26.1, 22.7, 14.1. Anal. Calcd. for $C_{75}H_{116}N_2O_6$: C, 78.90; H, 10.24; N, 2.45%. Found: C, 79.08; H, 10.13; N, 2.61%.

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References

[1] Sergerev, S., Pisula, W., and Geerts, Y. H. (2007). *Chem. Soc. Rev.*, *36*, 1902–1929.
[2] Tant, J., Geerts, Y. H., Lehmann, M., Cupere, V. D., Zucchi, G., Laursen, B. W., Bjrnholm, T., Lemaur, V., Mercq, V., Burquel, A., Hennebicq, E., Gardebien, F., Viville, P., Beljonne, D., Lazzaroni, R., and Cornil, J. (2005). *J. Phys. Chem. B.*, *109*, 20315–20323.
[3] Kumar, S. (2006). *Chem. Soc. Rev.*, *35*, 83–109.
[4] Stapff, J. H., Stumpflen, V., Wendorff, J. H., Spohn, D. B., and Mobius, D. (1997). *Liq. Cryst.*, *23*, 613–617.
[5] Barberá, J., Elduque, A., Giménez, R., Oro, L. A., and Serrano, J. L. (1996). *Angew. Chem., Int. Ed.*, *35*, 2832–2835.
[6] Chandrasekhar, S. (1982)."Liquid Crystals of Disc-like Molecules". In: G. H. Brown (Ed.), *Advances in Liquid Crystals*, Academic Press: New York, vol. 5, p. 47.
[7] Seo, S. H., Park, J. H., Tew, G. N., and Chang, J. Y. (2007). *Tetrahedron Lett.*, *48*, 6839–6844.
[8] Kishikawa, K., Oda, K., Aikyo, S., and Kohmoto, S. (2007). *Angew. Chem.*, *119*, 778–782.
[9] Serrette, A. G. and Swager, T. M. (1993). *J. Am. Chem. Soc.*, *115*, 8879–8880.
[10] Nguyen, H. T., Destrade, C., and Malthê, J. (1997). *Adv. Mater.*, *9*, 375–388.
[11] Goodby, J., Gray, G. W., Spiess, H. W., and Vill, V. (Eds.). (1998). *Handbook of Liquid Crystals*, Wiley-VCH: Weinheim, vol. 2B, p. 865.
[12] Eichhorn, S. H., Paraskos, A. J., Kishikawa, K., and Swager, T. M. (2002). *J. Am. Chem. Soc.*, *43*, 12742–12751.

[13] Gorecka, E., Pociecha, D., Mieczkowski, J., Matraszek, J., Guillon, D., and Donnio, B. (2004). *J. Am. Chem. Soc.*, *126*, 15946–15947.
[14] Kato, T., Mizoshita, N., and Kishimoto, K. (2006). *Angew. Chem.*, *118*, 44–74.
[15] Saez, I. M. and Goodby, J. W. (2005). *J. Mater. Chem.*, *15*, 26–40.
[16] Kato, T. (2002). *Science*, *295*, 2414–2418.
[17] Tschierske, C. (2001). *J. Mater. Chem.*, *11*, 2647–2671.
[18] Tschierske, C. (2001). *Annu. Rep. Prog. Chem. Sect. C*, *97*, 191–267.
[19] Kato, T. (1998). "Hydrogen-Bonded Systems". In: D. Demus, J. Goodby, G. W. Gray, H. W. Spiess, & V. Vill (Eds.), *Handbook of Liquid Crystals*, Wiley-VCH: Weinheim, vol. 2B, p. 969.
[20] Percec, V. (1997). In: P. J. Collings, & J. S. Patal (Eds.), *Handbook of Liquid Crystal Research*, Oxford University Press: New York, p. 259.
[21] Belloni, M., Manickam, M., & Preece, J. A. (2002). *Ferroelectrics*, *276*, 103–126.
[22] Su, L., Bao, C., Lu, R., Chen, Y., Xu, T., Song, D., Tan, C., Shi, T., and Zhao, Y. (2006). *Org. Biomol. Chem.*, *4*, 2591–2594.
[23] Kohlmeier, A. and Janietz, D. (2007). *Liq. Cryst.*, *34*, 289–294.
[24] Beltrán, E., Serrano, J. L., Sierra, T., and Giménez, R. (2010). *Org. Lett.*, *12*, 1404–1407.
[25] Donnio, B., Heinrich, B., Allouchi, H., Kain, J., Diele, S., Guillon, D., and Bruce, D. W. (2004). *J. Am. Chem. Soc.*, *126*, 15258–15268.
[26] Gorecka, E., Pociecha, D., Mieczkowski, J., Matraszek, J., Guillon, D., and Donnio, B. (2004). *J. Am. Chem. Soc.*, *126*, 15946–15947.
[27] Rossen, B. M., Wilson, C. J., Wilson, D. A., Peterca, M., Imam, M. R., and Percec, V. (2009). *Chem. Rev.*, *109*, 6275–6540.
[28] Majumdar, K. C., Chakravorty, S., Pal, N., and Sinha, R. K. (2009). *Tetrahedron*, *65*, 7998–8006.
[29] Majumdar, K. C., Mondal, S., De, N., Pal, N., Sinha, R. K., and Roy, B. (2010). *Tetrahedron Lett.*, *51*, 521–524.
[30] Majumdar, K. C., Mondal, S., Pal, N., and Sinha, R. K. (2009). *Tetrahedron Lett.*, *50*, 1992–1995.
[31] Majumdar, K. C., Mondal, S., and Sinha, R. K. (2010). *New. J. Chem.*, *34*, 1255–1260.
[32] Majumdar, K. C., Chakravorty, S., Sinha, R. K., and Pal, N. (2009). *Mol. Cryst. Liq. Cryst.*, *515*, 123–132.
[33] Majumdar, K. C., Ansary, I., and Roy, B. (2010). *Mol. Cryst. Liq. Cryst.*, *518*, 156–163.
[34] Majumdar, K. C., Pal, N., and Rao, N. V. S. (2006). *Liq. Cryst.*, *33*, 531–535.
[35] Grigoras, M. and Antonoaia, N. C. (2005). *Eur. Polym. J.*, *41*, 1079–1089.
[36] Sadashiva, B. K. and Raghunathan, V. A. (2003). *Pramana*, *61*, 219–229.
[37] Paraschiv, I., Giesbers, M., van Lagen, B., Grozema, F. C., Abellon, R. D., Siebbeles, L. D. A., Marcelis, A. T. M., Zuilhof, H., and SudhPlter, E. J. R. (2006). *Chem. Mater.*, *18*, 968–974.
[38] Ribeiro, A. C., Heinrich, B., Cruz, C., Nguyen, H. T., Diele, S., Schröder, M. W., and Guillon, D. (2003). *Eur. Phys. J. E.*, *10*, 143–151.
[39] CambridgeSoft. (2006). *Chem3D (version 10)*, CambridgeSoft: Cambridge, MA.
[40] Frisch, M. J., Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., Montgomery, Jr, J. A., Vreven, T., Kudin, K. N., Burant, J. C., Millam, J. M., Iyengar, S. S., Tomasi, J., Barone, V., Mennucci, B., Cossi, M., Scalmani, G., Rega, N., Petersson, G. A., Nakatsuji, H., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Klene, M., Li, X., Knox, J. E., Hratchian, H. P., Cross, J. B., Bakken, V., Adamo, C., Jaramillo, J., Gomperts, R., Stratmann, R. E., Yazyev, O., Austin, A. J., Cammi, R., Pomelli, C., Ochterski, J. W., Ayala, P. Y., Morokuma, K., Voth, G. A., Salvador, P., Dannenberg, J. J., Zakrzewski, V. G., Dapprich, S., Daniels, A. D., Strain, M. C., Farkas, O., Malick, D. K., Rabuck, A. D., Raghavachari, K., Foresman, J. B., Ortiz, J. V., Cui, Q., Baboul, A. G., Clifford, S., Cioslowski, J., Stefanov, B. B., Liu, G., Liashenko, A., Piskorz, P., Komaromi, I., Martin, R. L., Fox, D. J., Keith, T., Al-Laham, M. A., Peng, C. Y., Nanayakkara, A., Challacombe, M., Gill, P. M. W., Johnson, B., Chen, W., Wong, M. W., Gonzalez, C., and Pople, J. A. (2004). *Gaussian 03 (Revision C.02)*, Gaussian, Inc.: Wallingford, CT.