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Helical twisting behaviour of new chiral dopants with (S)-1, 2-propanediol units for nematic liquid crystals

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A novel series of chiral dopants synthesised from (S)-1, 2-propanediol and mesogenic carboxylic acids were characterised by Fourier transform infrared and ^{1}H nuclear magnetic resonance, and their helical twisting properties were investigated by doping the chiral dopants into a nematic liquid crystal host (SLC-1717). The results showed that the values of the molecular twisting power β were significantly dependent on the nature of the terminal substituents, terminal alkyl length and numbers of chiral centres in the molecular structure. Compared to compounds with electron-with-drawing groups (-NO_2, -F, -CF_3), the chiral compounds with terminal alkyl chains exhibited a higher β.

Keywords: chiral dopants; chiral nematic; pitch; molecular twisting power; liquid crystal

1. Introduction

Chirality is one of the most interesting and challenging subjects in the field of liquid crystals (LCs) for important technological applications [1, 2]. A chiral nematic liquid crystal (N*-LC) is formed when a nematic LC host is doped with a chiral dopant, and its helical structure is based on the chiral molecular structure [3]. On account of an integral part of the N*-LC for the chiral dopants, the design and synthesis of a new-style chiral dopant molecule has become a hot topic in the field of LC science [4–6]. Nowadays, much more investigation on the correlation between helical twisting sense and molecular structure has been carried out; the accumulated experimental data [7–10] and theoretical results [11, 12] show that the molecular shape of the additive and its conformational properties are the dominant factors that affect the value of HTP (the ability of a chiral dopant to generate a helical structure is measured as helical twisting power (HTP), βM (μm^{-1}), defined as the following equation, $\beta M = 1/P(cr)$. Here, P (μm) is the pitch of the chiral nematic phase, c the molar fraction of the dopant, and r the optical purity), but the category of chiral dopants was mainly chiral amino compounds [13, 14], binaphthyls [15], biphenyls [16] and certain metal complexes [17]. Recently, Mitov and Dessaud [18] investigated the polymorphism and optical behaviour of chiral dopants with a single (S)-1, 2-propanediol unit. We have also researched the helical twisting behaviour of chiral dopants containing a single chiral centre ((S)-1, 2-propanediol derivatives) [19, 20].

In this paper, in pursuit of a clearer understanding between the molecular structure and helical twisting behaviour of chiral dopants inducing N*-LCs, a novel series of optically active chiral (S)-1, 2-propanediol derivatives (C*n*TC, CSTC, CRDB) were synthesised and characterised. In addition, the influences of terminal alkyl chain length, type of substitutional group and numbers of the chiral centre on the helical twisting behaviour of the chiral dopants were investigated.

2. Experimental

2.1 Materials

The nematic LC host, SLC-1717 ($T_{N\text{-}I} = 91.8^\circ$C) was purchased from Shijiazhuang Yongsheng Huatsing Liquid Crystal Material Co., Ltd. and (S)-1, 2-propanediol (AR) was purchased from the Shanghai Darui Finechemical Company (China).

2.2 Synthesis

The synthesis routes of chiral 1, 2-propanediol derivatives are shown in Scheme 1.

2.2.1 Synthesis of compound C3TC

4-Hydroxy-benzoic acid ethyl ester (1.66 g, 10 mmol), NaOH (0.4 g, 10 mmol) and KI (0.166 g, 1 mmol) were dissolved in 20 mL 2-butanone, then the mixture was stirred for 20 min at 60°C. Furthermore, the butanone solution 10 mL of 1-bromo-propane (1.51 g, 10 mmol) was added dropwise while stirring. The reaction mixture was continuously stirred for 12 h at 95°C. After the solution was cooled to the surrounding

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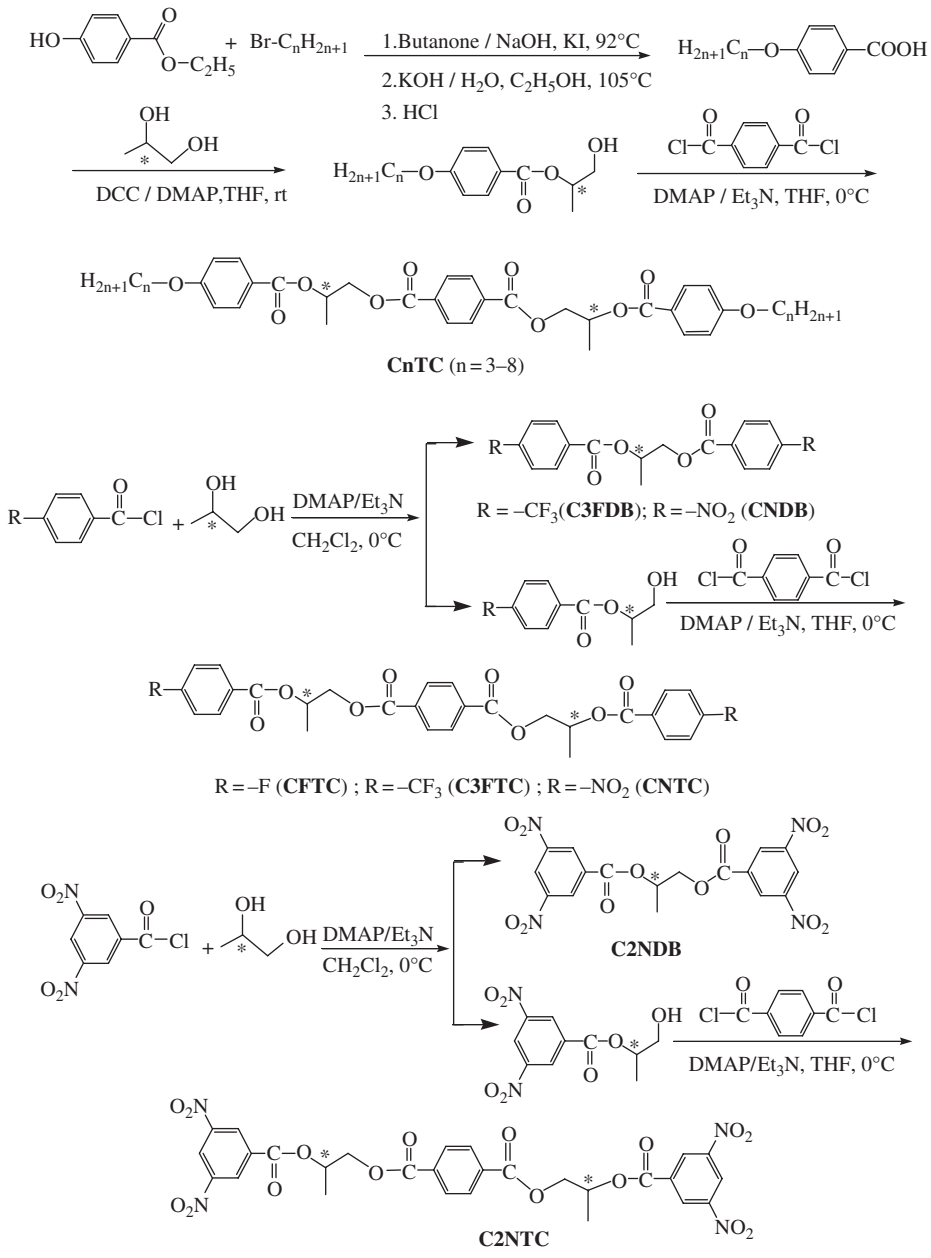

Scheme 1. The synthetic routes to chiral 1, 2-propanediol derivatives.

temperature, the precipitate was filtered off. The resulting solution was concentrated and then dissolved in 10 mL CH_2Cl_2, washed with 5% NaOH solution, 5% dilute hydrochloric acid and deionised water. The resulting solution was concentrated again and dissolved in 20 mL ethanol and mixed with 100 mL deionised water with KOH (0.56 g, 10 mmol). The reaction mixture was continuously stirred for 24 h at 105°C, then hydrochloric acid (37%) was added dropwise while stirring, at which point white precipitation appeared. The precipitate was filtrated to gain the crude product, which was then dried, and 2.08 g of white crystals were obtained by recrystallisation from ethanol twice. Yield: 88%.

(S)-1, 2-propanediol (0.91 g, 12 mmol) and 4-(dimethylamino) pyridine (DMAP) (0.25g, 2.0 mmol) were dissolved in 10 mL tetrahydrofuran (THF) (dry), and then added dropwise to a solution of 4-Propoxybenzoic acid (1.80 g, 10 mmol) and N,N′-dicyclohexylcarbodiimide (DCC) (2.48 g, 12 mmol) in 20 mL THF. The reaction mixture was continuously stirred at room temperature for 24 h. After the precipitate was filtered off, the resulting solution was evaporated under reduced pressure to remove the solvent. A solution of

the residue in CH_2Cl_2 was washed with distilled water, hydrochloric acid solution (1 mol L^{-1}) and potassium carbonate solution (1 mol L^{-1}) (3 × 30 ml), then the precipitate was filtered. Colourless liquid (1.42 g) was obtained by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 3/1). Yield: 59.7%. Fourier transform infrared (FT-IR) (KBr, cm^{-1}): 3445 (-OH), 2957, 2872 (-CH_3, -CH_2-), 1709 (C=O), 1607, 1508 (Ar-H). ^{1}H nuclear magnetic resonance (NMR) ($CDCl_3$, δ, ppm): 7.98–8.00 (4H, Ar-H), 4.32–4.34 (1H, C*-H), 4.01–4.18, 0.93–1.84 (12H, C*-CH_3, C*-CH_2-O-, alkyl-H), 2.03–2.17 (1H, -OH).

Terephthaloyl dichloride (0.51 g, 2.5 mmol) was dissolved in 20 mL THF (dry), then added dropwise to a solution of 4-Propoxy-benzoic acid 2-hydroxy-1-methyl-ethyl ester (1.19 g, 5 mmol), DMAP (0.12 g, 1 mmol) and triethylamine (Et_3N) (1 mL) in 20 mL THF under dry nitrogen. The reaction mixture was continuously stirred in an ice-water bath for 12 h with the reaction progress monitored by thin layer chromatography. After the removal of the solvent under reduced pressure, the residue in the CH_2Cl_2 solution was washed with dilute hydrochloric acid, 5% aqueous $NaHCO_3$ and deionised water, successively. After drying with anhydrous magnesium sulphate overnight, 0.94 g of white crystals was obtained by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 5/1). Yield: 61.8%. FT-IR (KBr, cm^{-1}): 3069, 2934, 2891, 1727, 1601, 1505, 1462, 1253, 1158, 1067, 854. ^{1}H NMR (CDCl3, δ, ppm): 8.07–8.08, 7.94–7.96, 6.87–6.89 (12H, Ar-H); 5.52–5.55 (2H, C*H); 4.46–4.50 (4H, C*-CH_2-O-); 1.37–1.41 (6H, C*-CH_3); 3.97–4.00, 1.77–1.81, 1.44–1.48, 0.91–0.94 (14H, alkyl-H).

2.2.2 C4TC: bis [1-(4-(butoxy) benzoyloxy)-2-yl] terephthalate

C4TC was synthesised by the analogous procedure used for C3TC in the yield of 45%. FT-IR (KBr, cm^{-1}): 3067, 2935, 2897, 1723, 1601, 1507, 1461, 1250, 1149, 1057, 852. ^{1}H NMR (500 MHz, CDCl3, δ, ppm): 7.94–7.98, 8.05–8.08, 6.87–6.90 (12H, Ar-H); 5.50–5.54 (2H, C*-H); 4.46–4.51 (4H, C*-CH_2-O-); 1.45–1.79 (6H, C*-CH_3); 3.98–4.02, 0.96–0.99 (18H, alkyl-H).

2.2.3 C5TC: bis [1-(4-(pentyloxy) benzoyloxy)-2-yl] terephthalate

C5TC was synthesised by the analogous procedure used for C3TC in the yield of 58%. FT-IR (KBr, cm^{-1}): 3078, 2931, 2871, 1721, 1605, 1510, 1465, 1260, 1169, 1098, 849. ^{1}H NMR (500 MHz, $CDCl_3$, δ, ppm): 8.05–8.09, 7.95–7.98, 6.87–6.90 (12H, Ar-H); 5.51–5.56 (2H, C*-H); 4.46–4.52 (4H, C*-CH_2-O-); 1.35–1.81 (6H, C*-CH_3); 3.97–4.00, 0.91–0.94 (22H, alkyl-H).

2.2.4 C6TC: bis [1-(4-(hexyloxy) benzoyloxy)-2-yl] terephthalate

C6TC was synthesised by the analogous procedure used for C3TC in the yield of 51%. FT-IR (KBr, cm^{-1}): 3072, 2931, 2893, 1724, 1601, 1506, 1461, 1255, 1152, 1065, 852. ^{1}H NMR (500 MHz, $CDCl_3$, δ, ppm): 8.05–8.09, 7.94–7.98, 6.87–6.90 (12H, Ar-H); 5.51–5.54 (2H, C*-H); 4.45–4.51 (4H, C*-CH_2-O-); 1.33–1.80 (6H, C*-CH_3); 3.97–4.00, 0.89–0.92 (26H, alkyl-H).

2.2.5 C7TC: bis [1-(4-(heptyloxy) benzoyloxy)-2-yl] terephthalate

C7TC was synthesised by the analogous procedure used for C3TC in the yield of 58%. FT-IR (KBr, cm^{-1}): 3062, 2934, 2892, 1722, 1601, 1502, 1461, 1254, 1152, 1061, 852. ^{1}H NMR (500 MHz, $CDCl_3$, δ, ppm): 8.05–8.07, 7.96–7.98, 6.88–6.90 (12H, Ar-H); 5.50–5.53 (2H, C*-H); 4.47–4.50 (4H, C*-CH_2-O-); 1.31–1.82 (6H, C*-CH_3); 3.98–4.01, 0.88–0.90 (30H, alkyl-H).

2.2.6 C8TC: bis [1-(4-(octyloxy) benzoyloxy)-2-yl] terephthalate

C8TC was synthesised by the analogous procedure used for C3TC in the yield of 56%. FT-IR (KBr, cm^{-1}): 3065, 2946, 2895, 1721, 1601, 1506, 1463, 1259, 1151, 1064, 855. ^{1}H NMR (500 MHz, $CDCl_3$, δ, ppm): 8.07–8.08, 7.94–7.96, 6.87–6.98 (12H, Ar-H); 5.51–5.55 (2H, C*-H); 4.46–4.49 (4H, C*-CH_2-O-); 1.28–1.81 (6H, C*-CH_3); 3.97–4.00, 0.87–0.90 (34H, alkyl-H).

2.2.7 Synthesis of compound CFTC

(S)-1, 2-propanediol (0.91 g, 12 mmol), DMAP (0.25 g, 2.0 mmol) and Et_3N (4 mL) were dissolved in 20 mL CH_2Cl_2 (dry), then added dropwise to a solution of 4-Fluoro-benzoyl chloride (1.59 g, 10 mmol) in 10 mL CH_2Cl_2 (2 h) under dry nitrogen. The reaction mixture was continuously stirred in an ice-water bath for 12 h with the reaction progress monitored by thin layer chromatography. After filtering the precipitate, the filtrate was washed with dilute hydrochloric acid, 5% aqueous $NaHCO_3$ and deionised water, successively. After drying with anhydrous magnesium sulphate overnight, 1.50 g of colourless liquid was obtained by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 3/1). Yield: 76%. FT-IR (KBr, cm^{-1}): 3441, 3080, 2978, 2888, 1720, 1603, 1505, 1453, 1277, 1158, 1117, 1090, 856, 767. ^{1}H NMR (500 MHz, $CDCl_3$, δ, ppm): 8.07–8.09 (2H, Ar-H), 7.12–7.14 (2H, Ar-H), 4.32–4.37 (H, C*-H), 4.16–4.22 (2H, -CH_2-), 2.02–2.04 (1H, -OH), 1.29–1.30 (3H, -CH_3).

4-Fluoro-benzoic acid 2-hydroxy-1-methyl-ethyl ester (0.99 g, 5 mmol), DMAP (0.125 g, 1.0 mmol), Et_3N (2 mL) and Terephthaloyl dichloride (0.51 g, 2.5 mmol) were dissolved in 20 mL THF (dry) under dry nitrogen. The reaction mixture was continuously stirred in an ice-water bath for 12 h with the reaction progress monitored by thin layer chromatography. After the removal of the solvent under reduced pressure, the residue in CH_2Cl_2 solution was washed with dilute hydrochloric acid, 5% aqueous $NaHCO_3$ and deionised water, successively. After drying with anhydrous magnesium sulphate overnight, 0.96 g of white crystals was obtained by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 6/1). Yield: 73%. FT-IR (KBr, cm^{-1}): 3072, 2987, 1726, 1603, 1505, 1456, 1409, 1263, 1155, 1103, 1018, 854, 767. ^1H NMR ($CDCl_3$, δ, ppm): 8.06–8.09, 8.01–8.04, 7.07–7.11 (12H, Ar-H); 5.53–5.58 (2H, C*H); 4.46–4.55 (4H, C*-CH_2-O-); 1.47–1.49 (6H, C*-CH_3).

2.2.8 *Synthesis of compound C3FTC*

C3FTC was synthesised by the analogous procedure used for CFTC in the yield of 78%. FT-IR (KBr, cm^{-1}): 3078, 2988, 1728, 1603, 1584, 1456, 1327, 1265, 1128, 1018, 864, 775. ^1H NMR ($CDCl_3$, δ, ppm): 8.11–8.15, 8.06–8.10, 7.66–7.69 (12H, Ar-H); 5.57–5.61 (2H, C*H); 4.51–4.60 (4H, C*-CH_2-O-); 1.49–1.51 (6H, C*-CH_3).

2.2.9 *Synthesis of compound CNTC*

CNTC was synthesised by the analogous procedure used for CFTC in the yield of 63%. FT-IR (KBr, cm^{-1}): 3056, 2986, 2880, 1726, 1607, 1530, 1462, 1348, 1290, 1175, 1080, 995, 845, 721. ^1H NMR ($CDCl_3$, δ, ppm): 8.25–8.28, 8.16–8.20, 8.05–8.08 (12H, Ar-H); 5.56–5.60 (2H, C*H); 4.50–4.59 (4H, C*-CH_2-O-); 1.49–1.51 (6H, C*-CH_3).

2.2.10 *Synthesis of compound C2NTC*

C2NTC was synthesised by the analogous procedure used for CFTC in the yield of 69%. FT-IR (KBr, cm^{-1}): 3101, 2986, 2884, 1729, 1607, 1545, 1460, 1344, 1265, 1169, 1103, 1018, 922, 823, 721. ^1H NMR ($CDCl_3$, δ, ppm): 8.08–8.11, 9.09–9.12, 9.19–9.21 (10H, Ar-H); 5.63–5.65 (2H, C*-H); 4.49–4.68 (4H, -CH2-); 1.54–1.55 (6H, -CH_3).

2.2.11 *Synthesis of compound C3FDB*

4-Trifluoromethyl-benzoyl chloride (2.09 g, 10 mmol), DMAP (0.25 g, 2.0 mmol) and Et_3N (4 mL) were dissolved in 20 mL THF (dry), then added dropwise to a solution of (S)-1, 2-propanediol (0.38 g, 5 mmol) in 10 mL THF (dry) under dry nitrogen. The reaction mixture was continuously stirred in an ice-water bath for 12 h with the reaction progress monitored by thin layer chromatography. After filtering the precipitate, the filtrate was washed with dilute hydrochloric acid, 5% aqueous $NaHCO_3$ and deionised water, successively. After drying with anhydrous magnesium sulphate overnight, 1.28 g of colourless liquid was obtained by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 3/1). Yield: 61%. FT-IR (KBr, cm^{-1}): 3076, 2990, 2957, 1730, 1585, 1516, 1411, 1327, 1267, 1130, 1018, 864, 775. ^1H NMR ($CDCl_3$, δ, ppm): 8.12–8.16, 7.68–7.71 (m, 8H, Ar-H), 5.57–5.63 (1H, C*-H), 4.51–4.61 (2H, -CH_2-), 1.1–1.52 (3H, -CH_3).

CNDB was synthesised by the analogous procedure used for C3FDB in the yield of 61%. FT-IR (KBr, cm^{-1}): 3047, 2958, 2882, 1722, 1604, 1549, 1462, 1346, 1253, 1165, 1080, 1007, 841, 721. ^1H NMR ($CDCl_3$, δ, ppm): 8.27–8.30, 8.17–8.21 (8H, Ar-H), 5.60–5.63 (1H, C*-H), 4.53–4.63 (2H, -CH_2-), 1.52–1.53 (3H, -CH_3).

2.3 *Preparation and characterisation of the twisting power of N*-LCs*

The nematic LC host of SLC-1717 and the desired chiral dopant were dissolved in acetone and then sonicated for at least 2.0 h to ensure that an even N*-LC mixture was obtained after removing the solvent.

The pitch, P, of the N*-LCs was measured by the Cano wedge technique [21]. In this measurement, a wedge-shaped cell with a wedge angle, α, was used and the inner surfaces of its two glass substrates were treated to provide a homogeneous orientation of LC molecules. After the sample was filled into the cell in the isotropic phase and then cooled to the N* phase, at a certain temperature a Grandjean–Cano texture formed with disclination lines separated by a distance, L. The pitch, P, is determined from $P = 2\alpha L$ at that temperature.

The twisting power is a measure of the ability of a chiral dopant to induce a N* phase in a nematic host. To characterise the twisting power of the synthesised chiral dopants, either the product pitch, P, or the molecular twisting power, $\beta = 1/PNv$, was used (Nv is the number density of the chiral dopant in mol m^{-3}, $Nv = c\rho/M$, c is the concentration of the chiral dopants in wt%, ρ is the density of SLC-1717 in 10^{-6} g m^{-3} and M is the molecular weight of the chiral dopants in g mol^{-1}) [18].

2.4 *Other characterisation*

FT-IR spectra of the intermediate and final compound were recorded on an E55×FRA106 FTIR/Raman spectrophotometer at frequencies ranging from 400 to 4000 cm^{-1}. ^1H NMR spectra were obtained on an AVANCZ 500 NMR spectrometer (with trimethylsilyl (TMS) as

the internal standard and $CDCl_3$ as the solvent). The optical textures were observed by a polarising microscope (POM, Olympus BX51) equipped with a hot stage calibrated to an accuracy of ±0.1°C (Linkam LK-600PM).

3. Results and discussion

3.1 Terminal alkyl chain length dependence of helical twisting behaviour

Figure 1 shows the temperature dependence of the molecular twisting power of C*n*TC (n = 3–8, c = 2.0 wt%). As can be seen, the chiral dopants with different terminal alkyl chain lengths exhibited similar temperature dependence of the induced helical structure, namely, decreasing absolute value β with increasing temperature. However, the decreasing degree was slightly different. In addition, no helix inversion could be found in the investigated temperature for C*n*TC. The helix inversion temperatures (T_{HI}), extrapolated from the fit linear of β curves, were 71.8°C for C3TC, 81.2°C for C5TC, 81.7°C for C7TC, 84.5°C for C4TC, 80.4°C for C6TC and 79.0°C for C8TC. This demonstrated that the T_{HI} varied with terminal alkyl chain length. For the C*n*TC (n = 3, 5, 7), the T_{HI} increased with the increasing terminal alkyl chain length, but the T_{HI} of chiral compounds C*n*TC (n = 4, 6, 8) decreased with the increasing terminal alkyl chain lengh. Furthermore, it should be noted that the absolute values of β increased with increasing terminal alkyl chain length as a whole. Typically, the β values at 40°C were –933.3 m^2 mol^{-1} for C3TC, –1018.8 m^2 mol^{-1} for C4TC, –1247.2 m^2 mol^{-1} for C5TC, –1436.6 m^2 mol^{-1} for C7TC and –1440.2 m^2 mol^{-1} for C8TC. The (+) sign indicates a right-handed and (–) sign a left-handed helical pitch. As reported, the twisting power is weakly dependent on the nature of the aliphatic chiral centre [22], and the increasing absolute values of β with increasing terminal alkyl chain length may result from greater anisometry of the molecular structure [18].

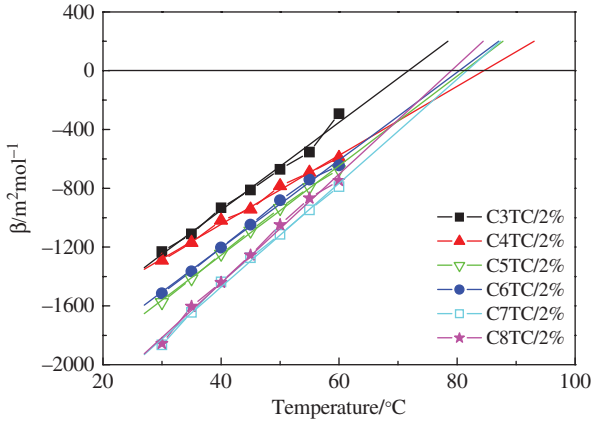

Figure 1. The temperature dependence of the molecular twisting power β of C*n*TC (n = 3–8).

3.2 Nature of the terminal substituents dependence of helical twisting behaviour

Figure 2 shows POM photos of the N*-LCs induced by C3FTC at different temperatures in the wedge-shaped cell (c = 5.0 wt%). As can be seen, the distance of parallel disclination lines increased with temperature increasing in the investigated temperature range from 26°C to 56°C. The homogeneous alignment of nematic LCs could be observed at about 56°C, with the transmitted light intensity of the cell changing periodically while rotating between the polariser and the analyser. That is to say, the pitch, P, of N*-LCs induced by C3FTC increased accordingly and became infinite at about 56°C, then a helix inversion occurred with the temperature variation. With temperature increasing further, the distance of parallel disclination lines decreased in the temperature range from 61°C

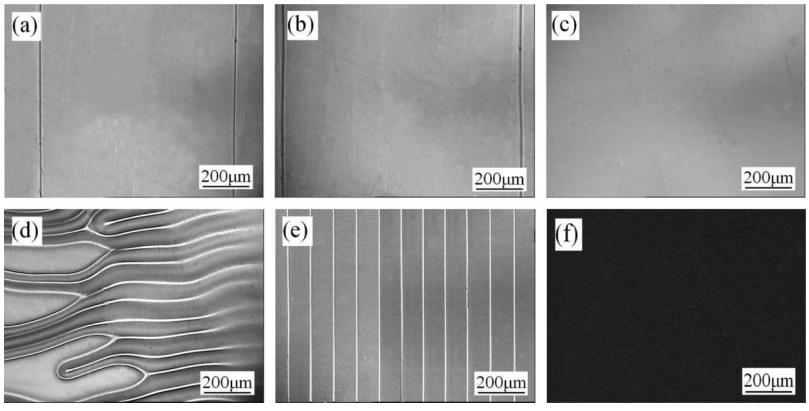

Figure 2. The POM photos of the N*-LC induced by C3FTC at different temperatures in the wedge-shaped cell: (a) 26°C; (b) 31°C; (c) 56°C; (d) 61°C; (e) 76°C; (f) 79°C.

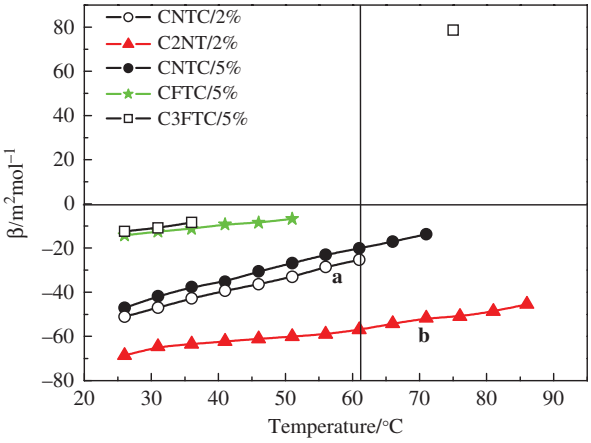

Figure 3. The temperature dependence of the molecular twisting power β of CNTC, C2NTC, CFTC and C3FTC.

to the temperature of the clearing point. This represented the pitch, P, with the opposite twisting sense decreasing with temperature increasing further.

Figure 3 shows the temperature dependence of the molecular twisting power of CNTC, C2NTC, CFTC and C3FTC. It can be seen that the molecular twisting power exhibited similar temperature dependence, namely decreasing absolute value β with increasing temperature. In addition, compared to C2NTC, with the highest molecular twisting power, C3FTC exhibited the lowest value among the four compounds, and the β varied slightly with the concentration of chiral dopants in wt% for the example of CNTC. For the compounds with the same concentration, the molecular twisting power of C2NTC was larger than that of CNTC. To our surprise, a helix inversion was found for C3FTC, which was different from the others (Figure 2).

The effect of substituents has been interpreted on the basis of their contribution to molecular polarisability, thus it was important to point out the role played by dispersive forces on the chirality transfer from the solute to the nematic solvent. Taking into account the aromatic structure of both the solutes and the solvents tested, attention should also be given to the arene–arene electrostatic interactions [23]. For the helix inversion phenomenon of C3FTC, the reason may be as follows: (a) the polarisability of trifluoromethylbenzene was the lowest in the series (apart from benzene), which brought forth weak dispersive forces; (b) the substituent CF_3- with the strongest ability for electron withdrawing affected the electron density on the aromatic ring and influenced both the polarisability and the charge distribution of the arenes, so it resulted in a weakening of the arene–arene electrostatic interactions; (c) the steric hindrance of CF_3- is the highest, which weakened the ability of chirality transfer.

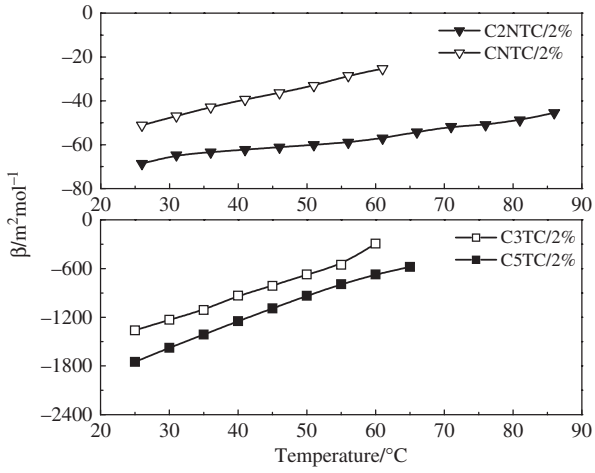

Figure 4. The temperature dependence of the molecular twisting power β of CNTC, C2NTC, C3TC and C5TC.

Figure 4 shows the temperature dependence of the molecular twisting power of C3TC, C5TC, CNTC and C2NTC (c = 2.0 wt%). As can be seen, all of the absolute values of β decreased with increasing temperature. C3TC and C5TC, with the electron withdrawing terminal groups, showed a larger molecular twisting power than that of CNTC or C2NTC which is a result of the increasing electrostatic arene–arene attraction with an increase of the electron density on the arene borne.

3.3 Chiral centre number dependence of helical twisting behaviour

Figure 5 shows the temperature dependence of the molecular twisting power of CNDB/CNTC and C3FDB/D3FTC (c = 5.0 wt%). As can be seen, CNTC showed a higher molecular twisting power

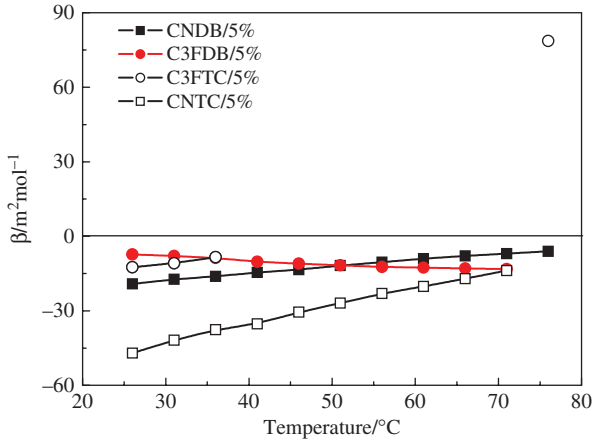

Figure 5. The temperature dependence of the molecular twisting power β of CNDB, CNTC, C3FDB and C3FTC.

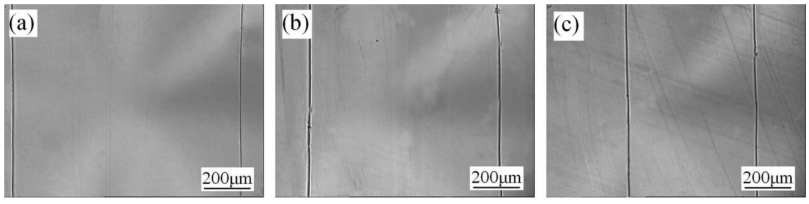

Figure 6. The POM photos of the N*-LC induced by C3FDB at different temperatures in the wedge-shaped cell: (a) 26°C; (b) 36°C; (c) 66°C.

compared to CNDB due to the higher concentration of chiral centres, and the curves of the β-temperature of the two compounds displayed a similar gradient, which indicated that the changes of molecular twisting power with increasing temperature were nearly the same; therefore, this explained that the disturbance between the two chiral centres was very weak and there was a plus property of the chiral centres on the helical twisting behaviour [18]. In addition, for the C3FDB and C3FTC, surprisingly, there was completely opposite temperature dependence of the molecular twisting power; the absolute value β of C3FDB showed positive temperature dependence, namely, it increased with increasing temperature, which was peculiar among all of the compounds we have synthesised.

Figure 6 shows POM photos of the N*-LCs induced by C3FDB at different temperatures in the wedge-shaped cell. As can be seen, the distance of parallel disclination lines decreased with temperature increasing in the investigated temperature range from 26°C to 66°C. That is to say, the pitch, P, of N*-LCs induced by C3FDB decreased accordingly, and eventually became infinite.

4. Conclusions

In conclusion, a novel series of chiral 1, 2-propanediol derivatives were synthesised and characterised. The helical twisting behaviour was investigated by doping the chiral dopants into a nematic LC host (SLC-1717). The results showed that all of the chiral dopants (except C3FDB) exhibited a similar temperature dependence of the helical twisting behaviour, typically decreasing absolute value β with increasing temperature. Surprisingly, C3FDB showed the opposite molecular twisting power–temperature dependence, namely, increasing absolute value β with increasing temperature. As the terminal alkyl chain length increased for the series of CnTC, the molecular twisting power increased, and an odd–even diversity was observed on the variety of T_{HI}. In addition, the nature of the terminal substituents affecting the electronic properties and the steric requirements of the chiral molecules could heavily affect the molecular twisting power. CnTC with electron-donating groups showed a larger molecular twisting power than that of CSTC with electron-withdrawing groups. A helix inversion was found for C3FTC, which was different from the other chiral compounds.

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