Supplementary material (ESI) for Journal of Materials Chemistry

Modulated general tilt structures in bent-core liquid crystals

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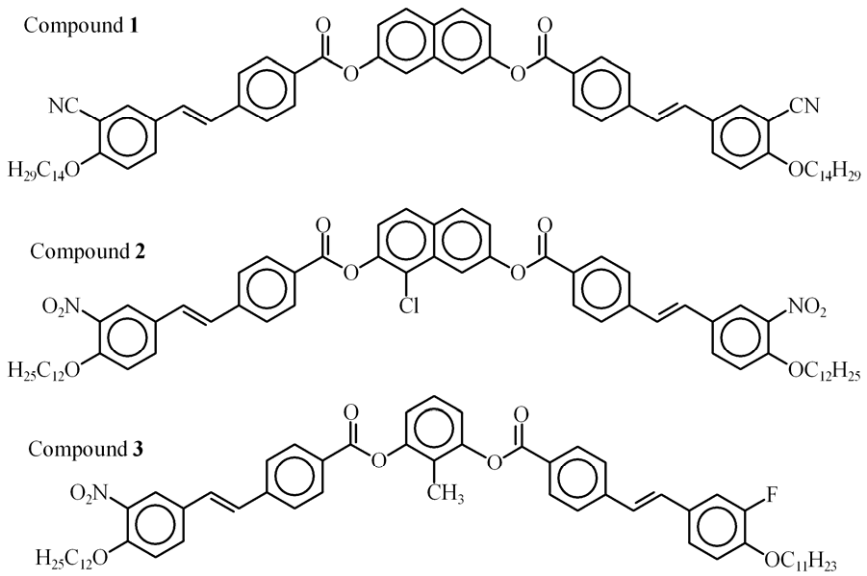
Experimental

Infrared (IR) spectra were obtained using a Nicolet Magna IR 500 spectrophotometer. NMR spectra were recorded on the Varian Unity Plus spectrometer operating at 200 MHz for ^{1}H-NMR and at 50 MHz for ^{13}C-NMR. Tetramethylsilane was used as an internal standard. Chemical shifts are reported in ppm. TLC analyses were performed on Merck 60 silica gel glass plated and visualized using iodine vapor. Column chromatography was carried out at atmospheric pressure using silica gel (100 - 200 mesh, Merck). A determined elemental composition of the synthesized compounds confirmed the expected molecular structure.

General procedure for synthesis of compound 1-3.



To 0.1 mol of central unit (2-methyl resorcine or 2,7-dihydroxynaphtalene) dissolved in anhydrous tetrahydrofurane 2 ml of triethylamine, 20mg of DMAP and 0.022 mol of corresponding acid chloride was added. The reaction mixture was heated under reflux during 8 hrs. Then solvents were evaporated under diminished pressure. The crude product was chromatographed on silica gel and eluted by dichloromethane. Yields were varying from 55 to 70%.

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Chemical analysis

Compound 1; $C_{70}H_{82}O_6N_2$, M=1046,

Elemental analysis: calc.: % C = 80.30, %H = 7.83, %N = 2.67;

found: % C = 80.11, %H = 7.95, %N = 2.55;

^1H NMR (200 MHz, $CDCl_3$, δ): 0.88 (t, 6H), 1.20-1.59 (m, 44H), 1.69-1.91 (m, 4H), 4.09 (t, 4H), 6.95 (d, 4H, J=8.8 Hz), 7.08 (d, 4H, J=7.8 Hz), 7.36 (dd, 2H, J_1=2.2 Hz, J_2=8.8Hz), 7.52-7.74 (m, 8H), 7.91 (d, 4H, J=8.8 Hz), 8.22 (d, 4H, J=8.4 Hz);

^{13}C NMR (50 MHz, $CDCl_3$, δ): 14.12, 22.69, 25.84, 28.88, 29.31, 29.36, 29.53, 29.60, 29.65, 31.92, 69.37, 102.58, 112.55, 116.18, 118.55, 121.21, 126.47, 127.37, 128.31, 128.99, 129.39, 129.53, 129.60, 130.75, 131.79, 132.49, 134.38, 142.06, 149.31, 160.57, 164.88,;

IR (KBr, cm^{-1}): 2922, 2852, 2225, 1725, 1600, 1499, 1274;

Compound 2; $C_{64}H_{73}O_{10}N_2Cl$, M=1064.5

Elemental analysis: calc.: % C = 72.14, %H = 6.85, %N = 2.63;

found: % C = 72.01, %H = 6.97, %N = 2.51;

^1H NMR (200 MHz, $CDCl_3$, δ): 0.88 (t, 6H, J=), 1.20-1.51 (m, 36H), 1.52-1.95 (m, 4H), 4.11 (t, 4H), 6.89-7.19 (m, 6H), 7.34-7.50 (m, 2H), 7.54-7.72 (m, 6H), 7.83 (d, 1H, J=9.0 Hz), 7.91 (d, 1H, J=9.0 Hz), 8.00 (d, 2H, J=1.8 Hz), 8.11 (d, 1H, J=2.2 Hz), 8.16-8.33 (m, 4H) ;

^{13}C NMR (50 MHz, $CDCl_3$, δ): 14.13, 22.70, 25.83, 28.93, 29.28, 29.35, 29.52, 29.59, 29.64, 31.92, 69.85, 69.98, 114.67, 115.83, 121.85, 122.03, 122.86, 123.44, 126.56, 127.76, 127.87, 128.20, 128.90, 128.97, 129.17, 129.91, 130.34, 130.81, 130.98, 132.06, 132.32, 140.02, 142.04, 142.20, 145.68, 152.25, 164.00, 164.80;

IR (KBr, cm^{-1}): 2925, 2854, 1726, 1600, 1511, 1275, 1240;

Compound 3; $C_{60}H_{72}O_8NF$, M=953

Elemental analysis: calc.: % C = 75.55, %H = 7.55, %N = 1.46;

found: % C = 75.43, %H = 7.63, %N = 1.35;

^1H NMR (200 MHz, $CDCl_3$, δ): 0.82-0.96 (m, 6H), 1.20-1.55 (m, 34H), 1.72-1.96 (m, 4H), 2.11 (s, 3H), 4.02-4.22 (m, 4H), 6.92-7.43 (m, 11H), 7.55-7.76 (m, 5H), 8.04 (d, 1H, J=2.0 Hz), 8.15-8.27 (m, 4H);

^{13}C *NMR* (50 MHz, $CDCl_3$, δ): 10.12, 14.14, 22.65, 22.73, 25.81, 25.82, 28.94, 29.17, 29.22, 29.28, 29.34, 29.36, 29.52, 29.59, 29.64, 31.81, 31.93, 69.47, 69.91, 113.51, 113.58, 114.61, 114.71, 119.93, 123.47, 123.54, 124.02, 126.59, 127.04, 127.94, 128.19, 128.91, 129.23, 129.88, 130.01, 147.58, 150.36, 152.28, 155.22, 164.31, 164.40;

IR (KBr, cm^{-1}): 2923, 2855, 1725, 1636, 1600, 1512, 1275, 1241;