Supporting Information

Diphenyltriacetylenes: Novel nematic liquid crystal materials and analysis of their nematic phase-transition and birefringence behaviours

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Spectral data

1,1'-(1,3,5-hexatriyne-1,6-diyl)bis[4-hexyloxybenzene] (OC6)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.5 Hz, Ar-H, 4H), 6.83 (d, *J* = 8.5 Hz, Ar-H, 4H), 3.96 (t, *J* = 6.6 Hz, Ar-O-CH_2, 4H), 1.78 (tt, *J* = 6.6 and 7.5 Hz, CH_2, 4H), 1.45 (tt, *J* = 7.0 and 7.5 Hz, CH_2, 4H), 1.37-1.30 (m, CH_2, 8H), 0.90 (t, *J* = 6.9 Hz, CH_3, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 134.6, 114.7, 112.6, 78.8, 73.5, 68.2, 66.4, 31.5, 29.0, 25.6, 22.6, 14.0 ppm; FT-IR (KBr) 2955, 2939, 2865, 2243, 2192, 1598, 1507, 1292, 1246, 1177 cm^{-1}.

1,1'-(1,3,5-hexatriyne-1,6-diyl)bis[4-heptyloxybenzene] (OC7)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.6 Hz, Ar-H, 4H), 6.84 (d, *J* = 8.6 Hz, Ar-H, 4H), 3.96 (t, *J* = 6.6 Hz, Ar-O-CH_2, 4H), 1.78 (tt, *J* = 6.6 and 7.5 Hz, CH_2, 4H), 1.44 (tt, *J* = 6.7 and 7.5 Hz, CH_2, 4H), 1.39-1.27 (m, CH_2, 12H), 0.93 (t, *J* = 6.7 Hz, CH_3, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 134.6, 114.7, 112.6, 78.8, 73.5, 68.2, 66.4, 31.7, 29.1, 29.0, 25.9, 22.6, 14.1 ppm; FT-IR (KBr) 2959, 2932, 2865, 2852, 2249, 2191, 1601, 1565, 1512, 1467, 1293, 1248, 1173 cm^{-1}.

1,1'-(1,3,5-hexatriyne-1,6-diyl)bis[4-octyloxybenzene] (OC8)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.8 Hz, Ar-H, 4H), 6.83 (d, *J* = 8.8 Hz, Ar-H, 4H), 3.96 (t, *J* = 6.6 Hz, Ar-O-CH_2, 4H), 1.78 (tt, *J* = 6.6 and 7.4 Hz, CH_2, 4H), 1.50-1.24 (m, CH_2, 20H), 0.89 (t, *J* = 6.7 Hz, CH_3, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 134.6, 114.7, 112.6, 78.8, 73.5, 68.2, 66.4, 31.8, 29.3, 29.2, 29.1, 26.0, 22.6, 14.1 ppm; FT-IR (KBr) 2922, 2866, 2851, 2249, 2189, 1597, 1562, 1513,

1467, 1291, 1251, 1178 cm^{-1}.

1,1'-(1,3,5-hexatriyne-1,6-diyl)bis[4-decyloxybenzene] (OC10)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 9.0 Hz, Ar-H, 4H), 6.83 (d, *J* = 9.0 Hz, Ar-H, 4H), 3.96 (t, *J* = 6.6 Hz, Ar-O-CH_2, 4H), 1.78 (tt, *J* = 6.6 and 7.5 Hz, CH_2, 4H), 1.44 (tt, *J* = 7.2 and 7.5 Hz, CH_2, 4H), 1.38-1.23 (m, CH_2, 24H), 0.88 (t, *J* = 6.8 Hz, CH_3, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 134.6, 114.7, 112.6, 78.8, 73.5, 68.2, 66.4, 31.9, 29.5, 29.5, 29.34, 29.30, 29.1, 26.0, 22.7, 14.1 ppm; FT-IR (KBr) 2952, 2920, 2864, 2846, 2247, 2191, 1599, 1567, 1514, 1476, 1467, 1294, 1254, 1171 cm^{-1}.

1,1'-(1,3,5-hexatriyne-1,6-diyl)bis[4-undecyloxybenzene] (OC11)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 9.0 Hz, Ar-H, 4H), 6.83 (d, *J* = 9.0 Hz, Ar-H, 4H), 3.96 (t, *J* = 6.6 Hz, Ar-O-CH_2, 4H), 1.78 (tt, *J* = 6.6 and 7.5 Hz, CH_2, 4H), 1.44 (tt, *J* = 7.1 and 7.5 Hz, CH_2, 4H), 1.36-1.23 (m, CH_2, 28H), 0.88 (t, *J* = 6.9 Hz, CH_3, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 134.6, 114.7, 112.6, 78.8, 73.5, 68.2, 66.4, 31.9, 29.60, 29.58, 29.54, 29.34, 29.32, 29.1, 26.0, 22.7, 14.1 ppm; FT-IR (KBr) 2949, 2924, 2869, 2849, 2247, 2193, 1602, 1567, 1510, 1473, 1465, 1290, 1251, 1173 cm^{-1}.

1,1'-(1,3,5-hexatriyne-1,6-diyl)bis[4-dodecyloxybenzene] (OC12)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.9 Hz, Ar-H, 4H), 6.83 (d, *J* = 8.9 Hz, Ar-H, 4H), 3.96 (t, *J* = 6.6 Hz, Ar-O-CH_2, 4H), 1.78 (tt, *J* = 6.6 and 7.4 Hz, CH_2, 4H), 1.44 (tt, *J* = 7.0 and 7.4 Hz, CH_2, 4H), 1.39-1.24 (m, CH_2, 32H), 0.88 (t, *J* = 6.8 Hz,

CH_3, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ160.7, 135.0, 115.1, 113.1, 79.2, 73.9, 68.6, 66.8, 32.3, 30.1, 30.04, 29.99, 29.96, 29.8 (29.8), 29.5, 26.4, 23.1, 14.5 ppm; FT-IR (KBr) 2953, 2921, 2868, 2849, 2246, 2189, 1599, 1567, 1510, 1475, 1466, 1294, 1253, 1173 cm^{-1}.

1,1'-(1,3,5-hexatriyne-1,6-diyl)bis[4-dodecyloxybenzene] (OC14)

^1H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.8 Hz, Ar-H, 4H), 6.83 (d, *J* = 8.8 Hz, Ar-H, 4H), 3.97 (t, *J* = 6.4 Hz, Ar-O-CH_2, 4H), 1.78 (tt, *J* = 6.4 and 7.6 Hz, CH_2, 4H), 1.44 (tt, *J* = 6.4 and 7.6 Hz, CH_2, 4H), 1.31-1.14 (m, CH_2, 40H), 0.88 (t, *J* = 6.4 Hz, CH_3, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 135.0, 115.1, 113.1, 79.2, 77. 6, 73.9, 68.6, 66.8, 32.3, 30.09 (30.09), 30.07, 29.98, 29.95, 29.8 (29.8), 29.5, 26.37, 23.1, 14.5 ppm; FT-IR (KBr) 2923, 2849, 2194, 1601, 1511, 1467, 1294, 1253, 1174 cm^{-1}.

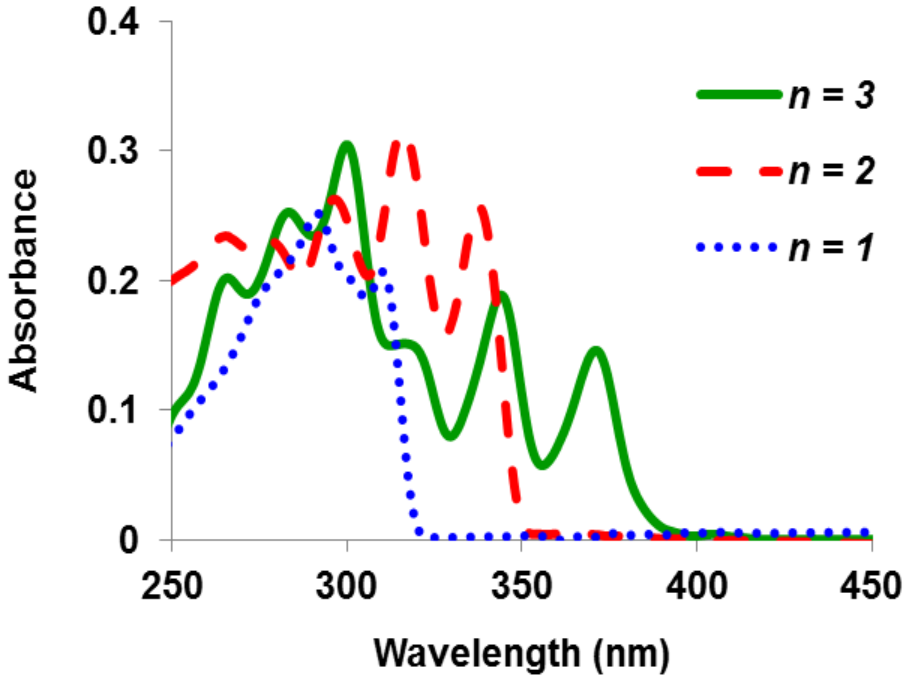

Fig. S1. UV-visible spectra of DPTA-OC6, DPDA-OC6 and DPA-OC6 in THF.

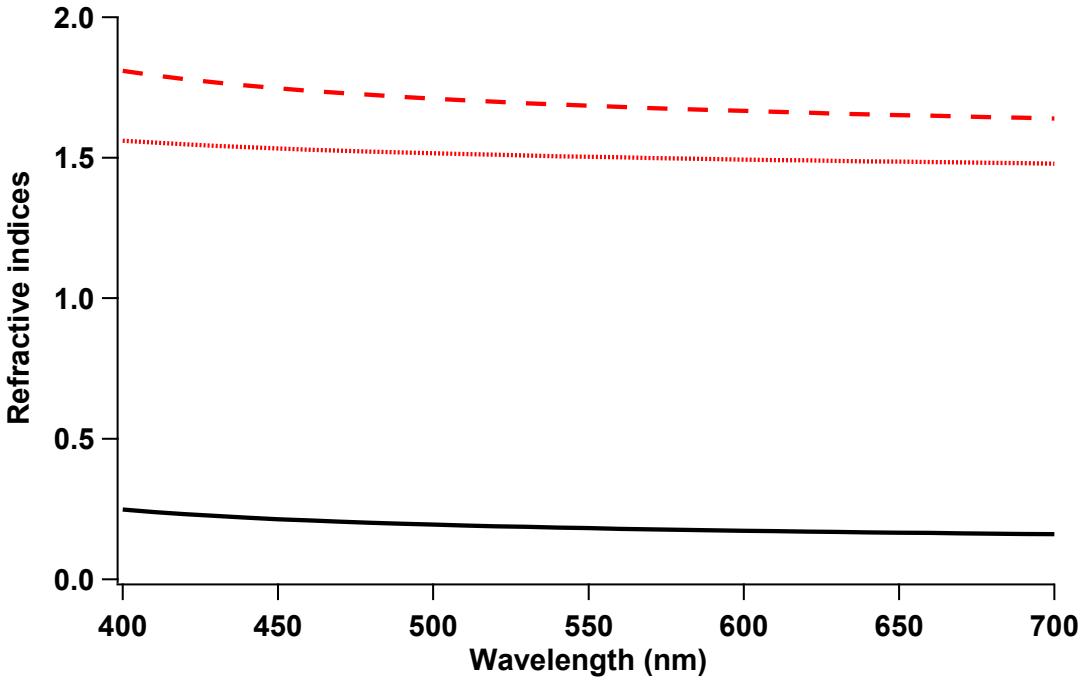

Fig. S2. Wavelength dispersion of refractive index parameters at 96 °C for DPA–OC6. Dashed line shows n_e, dotted line shows n_o and solid line shows Δn.

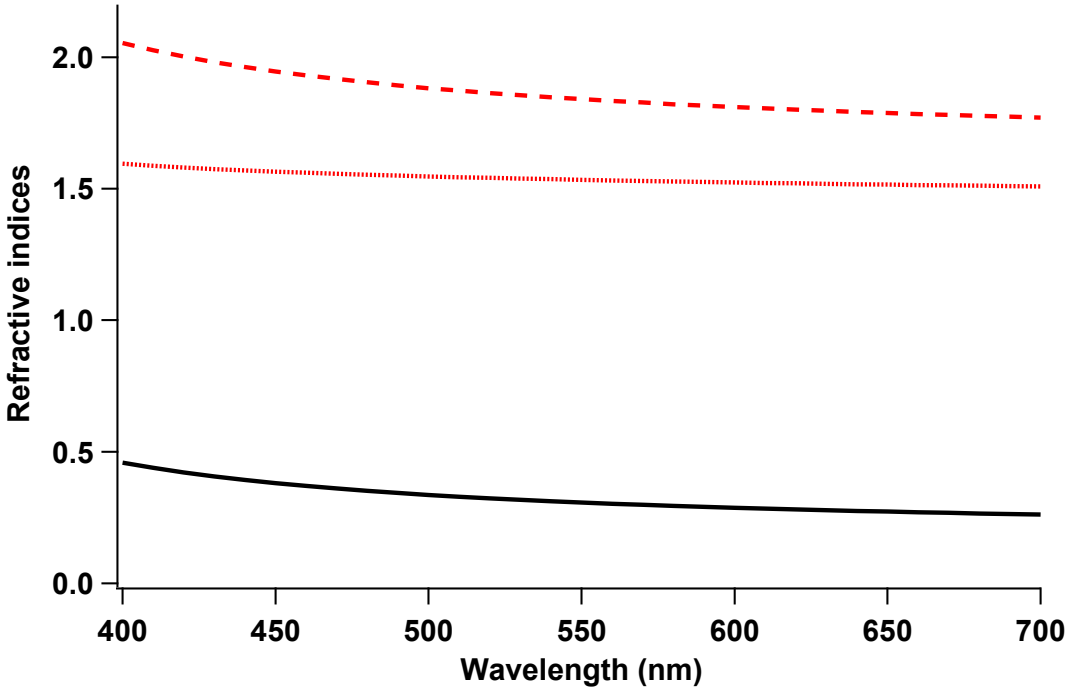

Fig. S3. Wavelength dispersion of refractive index parameters at 121 °C for DPDA–OC6. Dashed line shows n_e, dotted line shows n_o and solid line shows Δn.

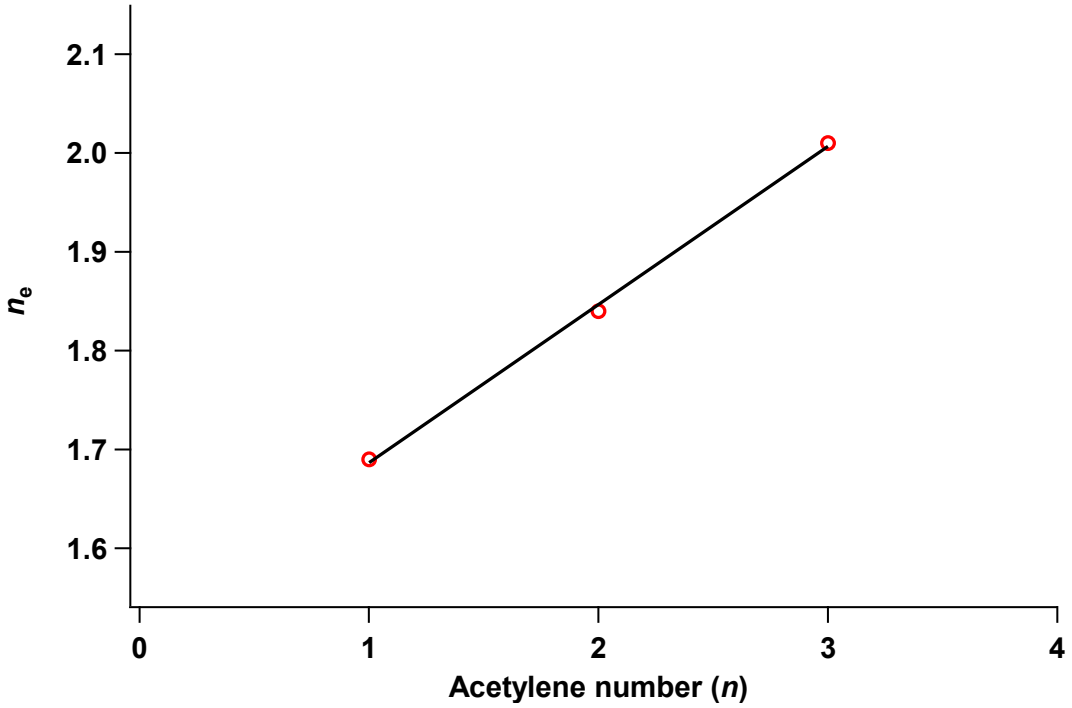

Fig. S4. The plots of n_e values against the number of acetylene units ($y = 0.160\ x + 1.53$, $R^2 = 0.999$).

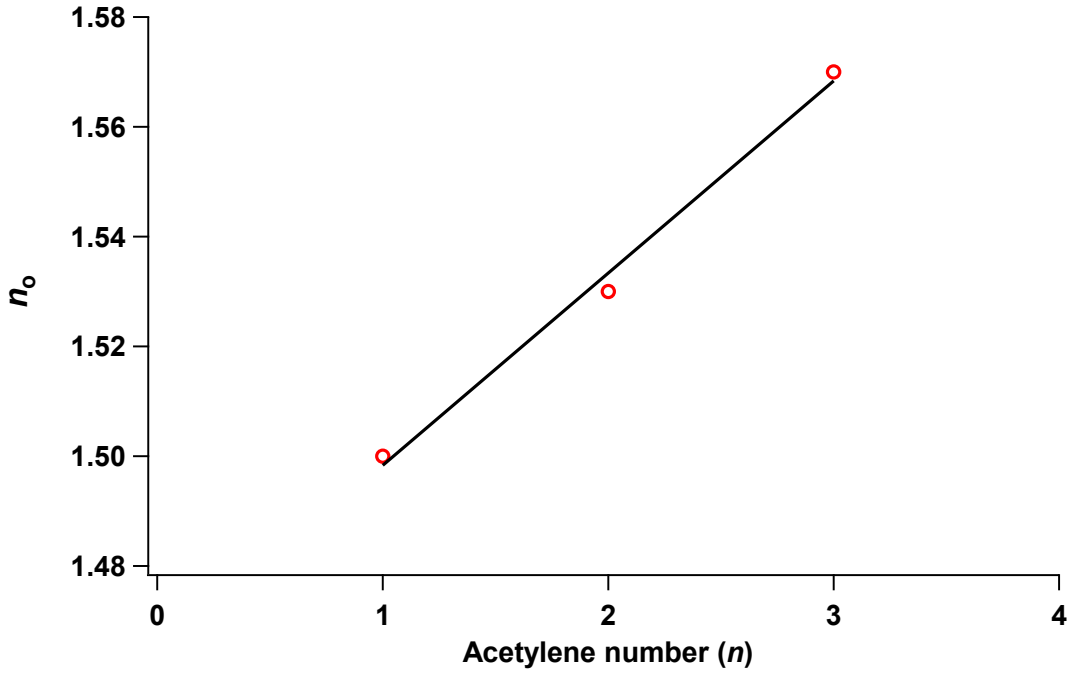

Fig. S5. The plots of n_o values against the number of acetylene units ($y = 0.0350x + 1.46$, $R^2 = 0.993$).