Supporting Information

Room-temperature liquid crystal of symmetric gallic trimer containing cyanuric core: Synthesis and mesomorphism

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1. General

All chemical reagents were obtained from commercial suppliers and used without further purification. The other organic solvents and inorganic reagents were purified according to standard anhydrous methods before use. TLC analysis was performed using pre-coated glass plates. ¹H NMR spectra were recorded in CDCl₃ on a Bruker-ARX 400 instrument at 30°C. Chemical shifts are reported in ppm, using tetramethylsilane (TMS) as internal standard. ESI-MS spectra were obtained from DECAX-30000 LCQ Deca XP mass spectrometer. Elemental analyses were performed at Vario EL III Elemental Analyzer. A polarized optical microscopy (Leica DMRX) was used along with a hot stage (Linkam THMSE 600) to examine phase transitions. Thermal analysis of the materials was carried out using a differential scanning calorimeter (DSC) (Thermal Analysis Q100) at a scanning rate of 10°C/min under N₂ atmosphere. X-ray diffraction (XRD) experiments were performed on SEIFERT-FPM (XRD7), using Cu Kα 1.5406 Å as the radiation source with 40 kV, 30 mA power.

Gallic derivative **2** with three long alkyl chains and its hydrazide derivative **3** was prepared according to the literature method (*J. Am. Chem. Soc.* 1997, 119, 1539). The 1,3,5-triazine-based derivatives **6**, **9** and **11** with one, two and three aldehyde groups were synthesized in high yields with the literature method (*Liq. Cryst.* **2012**, 39, 1368-1374.).

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2. The synthetic procedure of compounds 7, 10 and 12

Scheme S1 The synthetic routes of compounds **7**, **10**, **12**

2.1 Synthesis of gallic monomer with *cyanuric core 7*

Under N₂ atmosphere, the mixture of triazine derivative **6** (0.0575 g, 0.15 mmol) and gallic hydrazide **3** (0.104 g, 0.15 mmol) was refluxed in 20 mL of methanol/CHCl₃(3:1, V/V) by using 0.10 mL of acetic acid as catalyst. After reaction overnight, TLC detection indicated the disappearance of starting materials. Then the solvent was evaporated under reduced pressure. The residue was treated by 10 mL of methanol and precipitate was formed. The precipitate was filtered and washed by small amounts of methanol for three times. After vacuum dryness, compound **7** was obtained as white solid in 84% yield. Compound **7**: FT-IR(KBr), ν/cm^{-1} : 3414, 2924, 2855, 1632, 1578, 1487, 1446, 1341, 1232, 1205, 1114, 809; ¹H NMR (400 MHz, CDCl₃) δ (ppm): 0.89 (t, J = 8.4Hz, 9H, CH₃), 1.25-1.80(m, 60H, C₁₀H₂₀), 3.60-4.01 (m, 6H,

ArOCH₂), 6.70-7.41(m, 18H, ArH and ArNH), 8.35 (s, 1H, CH=N), 9.58(s, 1H, CONH). MS(*m/z*) (%): 1053.7(M⁺, 100). Anal. Calcd for C₆₅H₉₅N₇O₅: C 74.04, H 9.08, N 9.30; found C 74.02, H 9.09, N 9.28.

2.2 Synthesis of gallic dimer with *cyanuric core 10*

Under N₂ atmosphere, the mixture of triazine derivative **9** (0.0412 g, 0.1 mmol) and gallic hydrazide **3** (0.138 g, 0.2 mmol) was refluxed in 20 mL of methanol/CHCl₃(3:1, V/V) by using 0.15 mL of acetic acid as catalyst for 6 h, TLC detection indicated the disappearance of starting materials. Then the solvent was evaporated under reduced pressure and the residue was treated by 10 mL of methanol to afford precipitate. The precipitate was filtered and washed by small amounts of MeOH for three times. After vacuum dryness, compound **10** was obtained as pale solid in 88% yield. Compound **10**: FT-IR(KBr), ν/cm^{-1} : 3417, 2924, 2855, 1618, 1573, 1491, 1423, 1373, 1209, 1110, 809; ¹H NMR (400 MHz, CDCl₃) δ (ppm): 0.97(t, *J* = 8.0 Hz, 18H, CH₃), 1.26-1.84(m, 120H, C₁₀H₂₀), 3.63-4.02 (m, 12H, ArOCH₂), 6.69-7.38 (m, 18H, ArH and ArNH), 8.41(s, 2H, CONH), 8.66 (bs, 2H, CH=N). MS(*m/z*) (%): 1754.3(M⁺, 100). Anal. Calcd for C₁₀₉H₁₇₂N₈O₁₀: C 74.61, H 9.88, N 6.39; found C 74.64, H 9.84, N 6.38.

2.3 Synthesis of gallic trimer with *cyanuric core 12*

Under N₂ atmosphere, the mixture of triazine derivative **11** (0.0221 g, 0.05 mmol) and gallic hydrazide **3** (0.104 g, 0.15 mmol) was refluxed in 30 mL of methanol/CHCl₃(3:1, V/V) by using 0.2 mL of acetic acid as catalyst. TLC detection indicated the disappearance of starting materials in 12 h. Then the solvent was evaporated under reduced pressure. The residue was treated by 10 mL of methanol to afford white precipitate. The precipitate was filtered and washed by some methanol for three times. After vacuum dryness, compound **12** was obtained as pale soft solid in yield of 80%. Compound **12**: FT-IR(KBr), ν/cm^{-1} : 3414, 2924, 2860, 1646, 1564, 1491, 1364, 1205, 1114, 841; ¹H NMR (400 MHz, CDCl₃) δ (ppm): 0.87(s, 27H, CH₃), 1.25-1.83(m, 180H, C₁₀H₂₀), 3.64-4.05 (m, 18H, ArOCH₂), 6.88~7.94(m, 18H, ArH), 8.51 (bs, 3H, CH=N), 8.90 (bs, 3H, CONH). MS(*m/z*) (%): 2453.8(M⁺, 100). Anal. Calcd for C₁₅₃H₂₄₉N₉O₁₅: C 74.86, H 10.22, N 5.14; found C 74.84, H 10.26, N 5.10.

Figure S1 The IR spectra of compounds **7**, **10**, **12**

Figure S2 The ^1H NMR spectrum of compound **7**

Figure S3 The ¹H NMR spectrum of compound 10

Figure S4 The ¹H NMR spectrum of compound 12

Figure S5 The ESI-MS spectrum of compound **7**

Figure S6 The ESI-MS spectrum of compound **10**

Figure S7 The ESI-MS spectrum of compound **12**