Supporting Information

Polycatenar liquid crystals based on bent-shaped chalcone and cyanopyridine molecules.

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Experimental

1. Synthesis

(E)-1,3-bis(4-hydroxyphenyl)prop-2-en-1-one **2**

BF₃OEt₂ (10 mmol) was added gradually to a solution of 4-hydroxyacetophenone (20 mmol) and 4-hydroxybenzaldehyde (20 mmol) in dioxane (4 mL), and stirred at room temperature for 2 h. The mixture was added to cold ethyl acetate and the precipitate formed was filtered and washed with water. The resulting solid was purified by column chromatography using hexane/EtOAc 1:1 (v/v), affording a yellow solid. Yield: 46%. M.p.: 200.2-202.4 °C. IR (KBr) ν_{max} cm⁻¹: 3298, 3016, 2802, 2684, 2604, 1643, 1603, 1584, 1562, 1509, 1446, 1344, 1280, 1217, 1262, 1113, 1032, 974, 815, 609, 534, 516.

^1H NMR (400 MHz, DMSO- d_6) δ ppm: 10.36 (*br*, 1 H, O-H), 10.06 (*br*, 1 H, O-H), 8.05 (*d*, 2 H, $J = 8.6$ Hz, Ar-H), 7.62 (*d*, 2 H, $J = 8.6$ Hz, Ar-H), 7.68 (*d*, 1 H, $J = 15.6$ Hz, =C-H), 7.63 (*d*, 1 H, $J = 15.6$ Hz, =C-H), 6.89 (*d*, 2 H, $J = 8.6$ Hz, Ar-H), 6.84 (*d*, 2 H, $J = 8.6$ Hz, Ar-H). ^{13}C NMR (100 MHz, DMSO- d_6): δ ppm = 187.09, 161.95, 159.87, 143.23, 131.00, 130.80, 129.48, 126.03, 118.54, 115.82, 115.34.

2. NMR spectra of compounds Ia-c and IIa-d

a)

b)

Figure S1. (a) ¹H NMR spectrum of compound Ia (CDCl₃) and (b) ¹³C NMR spectrum of compound Ia (CDCl₃).

a)

b)

Figure S2. (a) ¹H NMR spectrum of compound Ib (CDCl₃) and (b) ¹³C NMR spectrum of compound Ib (CDCl₃).

a)

b)

Figure S3. (a) ¹H NMR spectrum of compound Ic (CDCl₃) and (b) ¹³C NMR spectrum of compound Ic (CDCl₃).

a)

b)

Figure S4. (a) ¹H NMR spectrum of compound IIa (CDCl₃) and (b) ¹³C NMR spectrum of compound IIa (CDCl₃).

a)

b)

Figure S5. (a) ¹H NMR spectrum of compound IIb (CDCl₃) and (b) ¹³C NMR spectrum of compound IIb (CDCl₃).

Figure S6. (a) ¹H NMR spectrum of compound IIc (CDCl₃) and (b) ¹³C NMR spectrum of compound IIc (CDCl₃).

a)

b)

Figure S7. (a) ¹H NMR spectrum of compound IIId (CDCl₃) and (b) ¹³C NMR spectrum of compound IIId (CDCl₃).

3. MS Spectra

Figure S8. Mass Spectra of compound Ia.

Figure S9. Mass spectra of compound Ib.

Figure S10. Mass spectra of compound Ic.

Figure S11. Mass spectra of compound IIa.

Figure S12. Mass spectra of compound IIb.

Figure S13. Mass spectra of compound IIc.

Figure S14. Mass spectra of compound IId.

4. DSC Thermograms

Figure S15. Thermograms obtained by DSC analysis showing the second cycle of heating and cooling (10 °C min⁻¹) in nitrogen atmosphere for compound Ia.

Figure S16. Thermograms obtained by DSC analysis showing the second cycle of heating and cooling ($10\text{ }^{\circ}\text{C min}^{-1}$) in nitrogen atmosphere for compound Ib.

Figure S17. Thermograms obtained by DSC analysis showing the second cycle of heating and cooling ($10\text{ }^{\circ}\text{C min}^{-1}$) in nitrogen atmosphere for compound IIa.

Figure S18. Thermograms obtained by DSC analysis showing the second cycle of heating and cooling ($10\text{ }^{\circ}\text{C min}^{-1}$) in nitrogen atmosphere for compound IIb.

Figure S19. Thermograms obtained by DSC analysis showing the second cycle of heating and cooling ($10\text{ }^{\circ}\text{C min}^{-1}$) in nitrogen atmosphere for compound IIId.

5. TGA curves

Figure S20. Thermogram of compound Ia.

Figure S21. Thermogram of compound Ib.

Figure S22. Thermogram of compound Ic.

Figure S23. Thermogram of compound IIa.

Figure S24. Thermogram of compound IIb.

Figure S25. Thermogram of compound IIc.

Figure S26. Thermogram of compound IIId.