

Supporting information

Birefringence and photoluminescence properties of diphenylacetylene-based liquid crystal dimers

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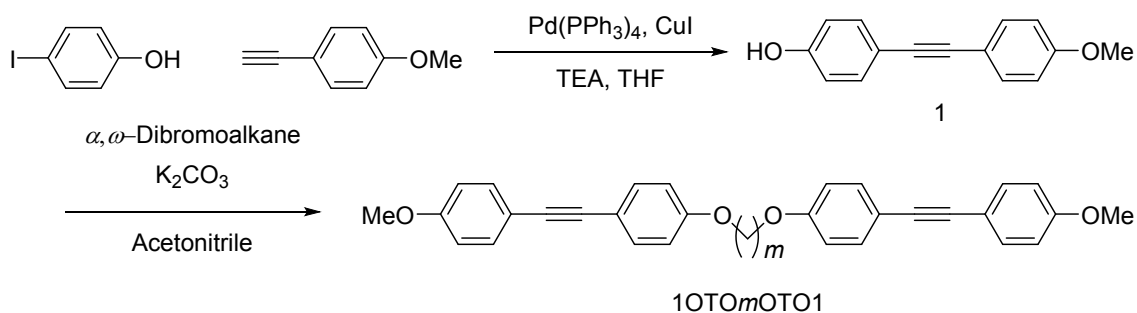
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Synthesis and characterization

All of the dimer homologues series were synthesized according to the Scheme S1 and procedures described in the manuscript. The quantities of the chemicals used for the

syntheses, each yield and molecular structural characterization data confirmed based on ^1H NMR (on a JEOL LNM-EX 400) measurements are described below, except for those for 1OTO9OTO1 depicted in the manuscript.



Scheme S1. synthetic pathway for 1OTOmOTO1 homologues.

1,5-Bis{4'-[(4-methoxyphenyl)ethynyl]phenoxy}pentane (1OTO5OTO1)

Yield: 76% (0.134 g). ^1H NMR (CDCl_3 , 400 MHz) δ 7.45 (d, 4H), 7.44 (d, 4H), 6.87 (d, 4H), 6.86 (d, 4H), 4.01 (t, 4H), 3.82 (s, 6H), 1.87 (tt, 4H), 1.67 (tt, 2H) ppm.

1,6-Bis{4'-[(4-methoxyphenyl)ethynyl]phenoxy}hexane (1OTO6OTO1)

Yield: 64% (0.123 g). ^1H NMR (CDCl_3 , 400 MHz) δ 7.45 (d, 4H), 7.44 (d, 4H), 6.89 (d, 4H), 6.86 (d, 4H), 3.99 (t, 4H), 3.83 (s, 6H), 1.83 (tt, 4H), 1.60-1.50 (m, 4H) ppm.

1,7-Bis{4'-[(4-methoxyphenyl)ethynyl]phenoxy}heptane (1OTO7OTO1)

Yield: 74% (0.189 g). ^1H NMR (CDCl_3 , 400 MHz) δ 7.44 (d, 4H), 7.43 (d, 4H), 6.86 (d, 4H), 6.85 (d, 4H), 3.97 (t, 4H), 3.82 (s, 6H), 1.81 (tt, 4H), 1.60-1.39 (m, 4H) ppm.

1,8-Bis{4'-[(4-methoxyphenyl)ethynyl]phenoxy}octane (1OTO8OTO1)

Yield: 55% (0.108 g). ^1H NMR (CDCl_3 , 400 MHz) δ 7.44 (d, 4H), 7.43 (d, 4H), 6.86 (d, 4H), 6.85 (d, 4H), 3.97 (t, 4H), 3.82 (s, 6H), 1.80 (tt, 4H), 1.52-1.37 (m, 8H) ppm. ^{13}C NMR (CDCl_3 , 100 MHz) δ ppm.

1,10-Bis{4'-[(4-methoxyphenyl)ethynyl]phenoxy}decane (1OTO10OTO1)

Yield: 75% (0.117 g). ^1H NMR (CDCl_3 , 400 MHz) δ 7.45 (d, 4H), 7.43 (d, 4H), 6.87 (d, 4H), 6.86 (d, 4H), 3.96 (t, 4H), 3.82 (s, 6H), 1.79 (tt, 4H), 1.52-1.41 (m, 4H) 1.40-1.31 (m, 8H) ppm. ^{13}C NMR δ (CDCl_3 , 100 MHz).

1,11-Bis{4'-[(4-methoxyphenyl)ethynyl]phenoxy}undecane (1OTO11OTO1)

Yield: 68% (0.137 g). ^1H NMR (CDCl_3 , 400 MHz) δ 7.44 (d, 4H), 7.42 (d, 4H), 6.86 (d, 4H), 6.85 (d, 4H), 3.96 (t, 4H), 3.82 (s, 6H), 1.78 (tt, 4H), 1.45 (tt, 4H) 1.40-1.27 (m, 10H) ppm.

1,12-Bis{4'-[(4-methoxyphenyl)ethynyl]phenoxy}dodecane (1OTO12OTO1)

Yield: 67% (0.111 g). ^1H NMR (CDCl_3 , 400 MHz) δ 7.44 (d, 4H), 7.43 (d, 4H), 6.86 (d, 4H), 6.85 (d, 4H), 3.96 (t, 4H), 3.82 (s, 6H), 1.78 (tt, 4H), 1.45 (tt, 4H), 1.41-1.24 (m, 12H) ppm.

POM images

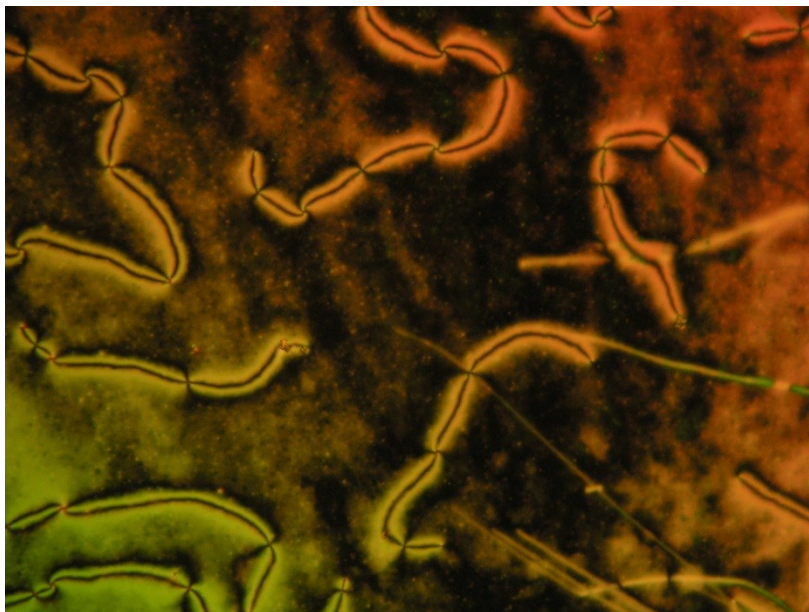


Fig. S1. POM image of N phase at 170 °C of 1OTO5OTO1.

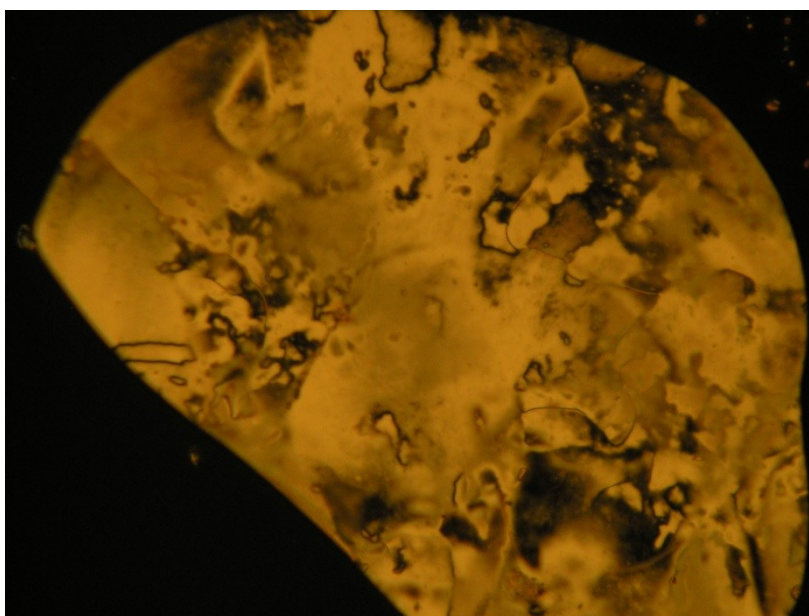


Fig. S2. POM image of N phase at 210 °C of 1OTO6OTO1.

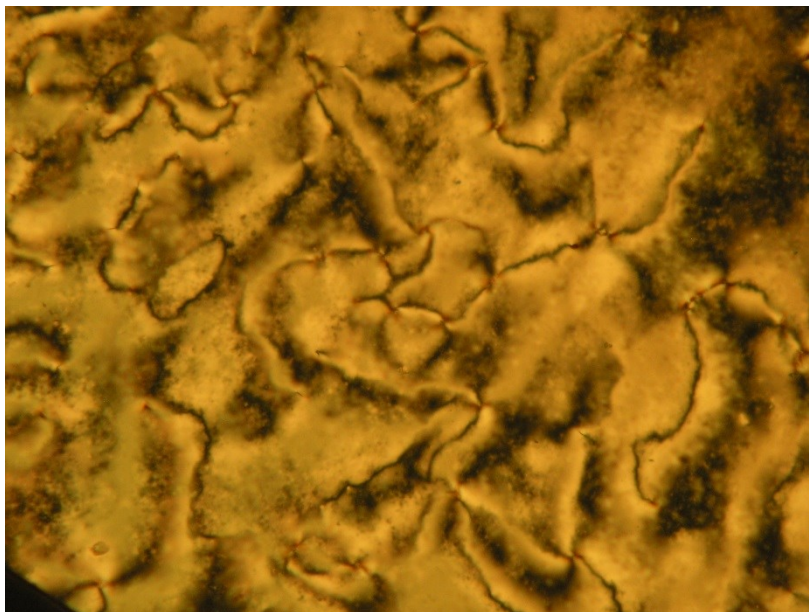


Fig. S3. POM image of N phase at 160 °C of 1OTO7OTO1.

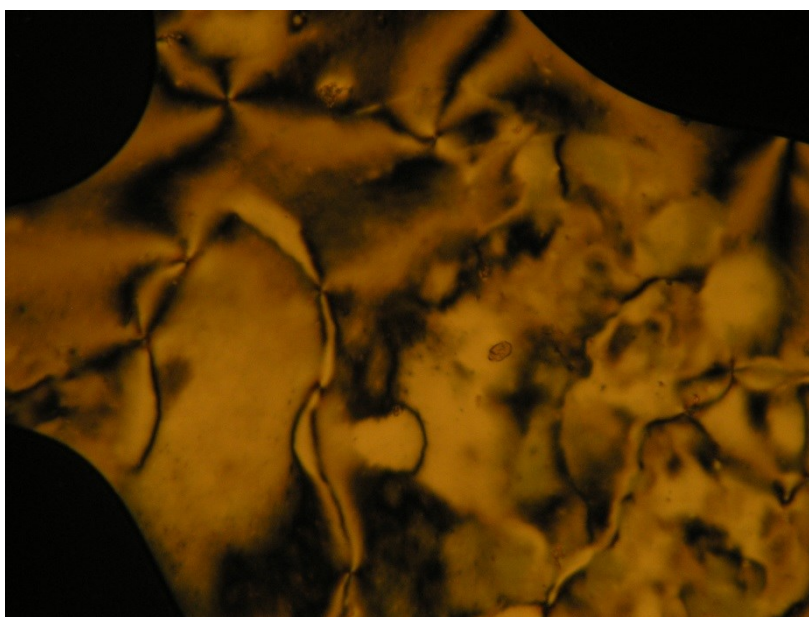


Fig. S4. POM image of N phase at 170 °C of 1OTO8OTO1.

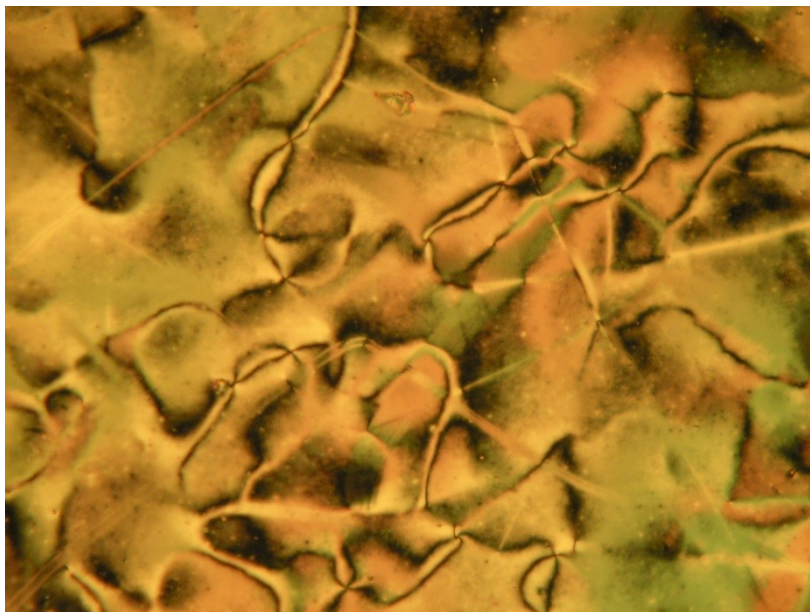


Fig. S5. POM image of N phase at 105 °C of 1OTO9OTO1.

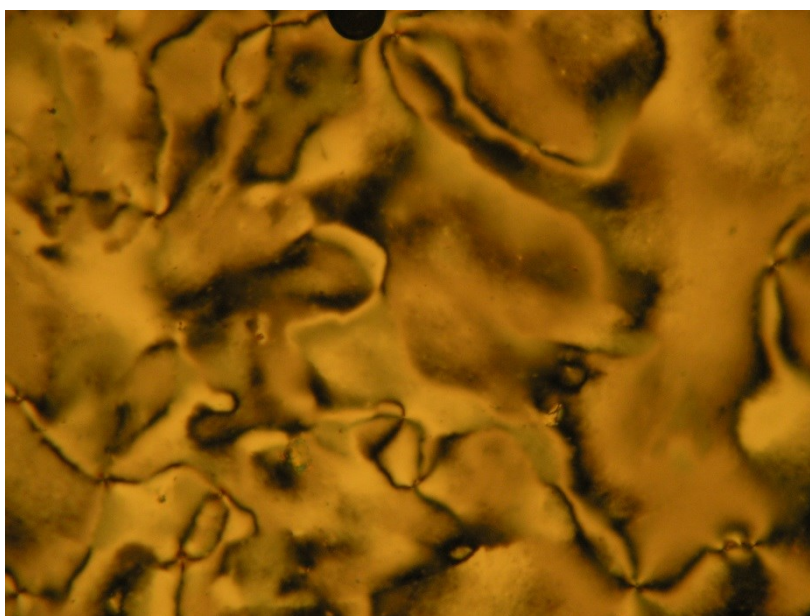


Fig. S6. POM image of N phase at 180 °C of 1OTO10OTO1.

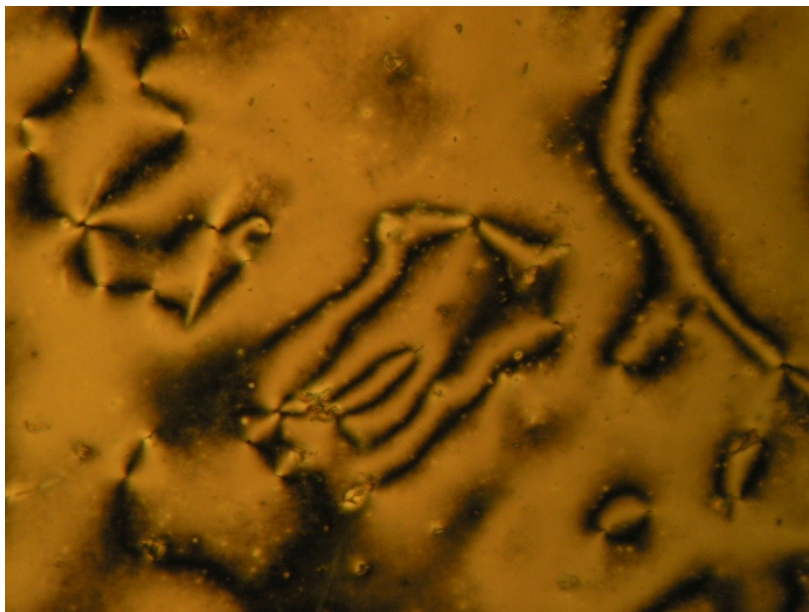


Fig. S7. POM image of N phase at 105 °C of 1OT11OTO1.

DSC measurements

The DSC thermograms are based basically on second heating and first cooling.

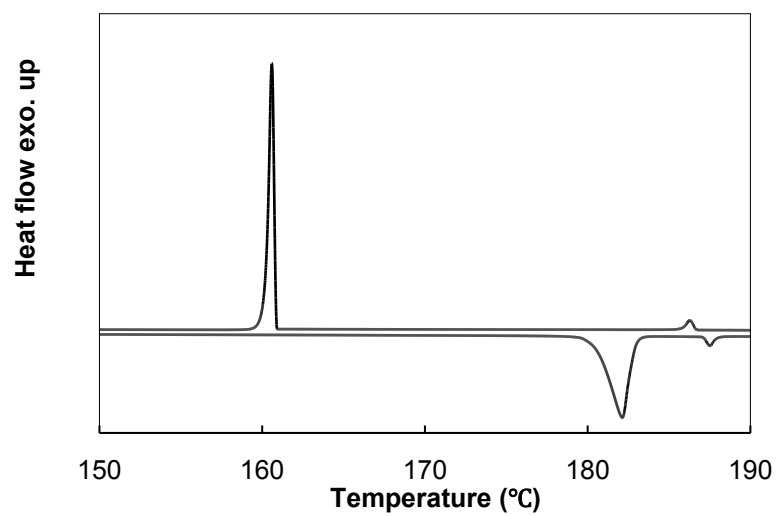


Fig. S8. DSC thermogram of 1OTO5OTO1.

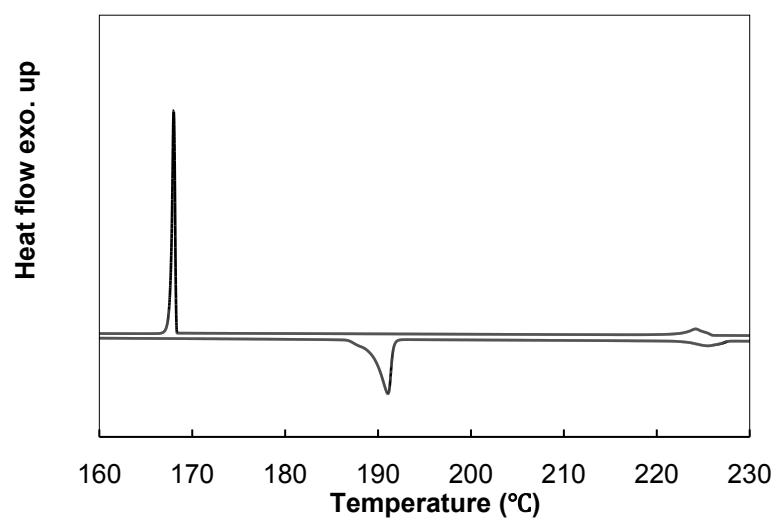


Fig. S9. DSC thermogram of 1OTO6OTO1.

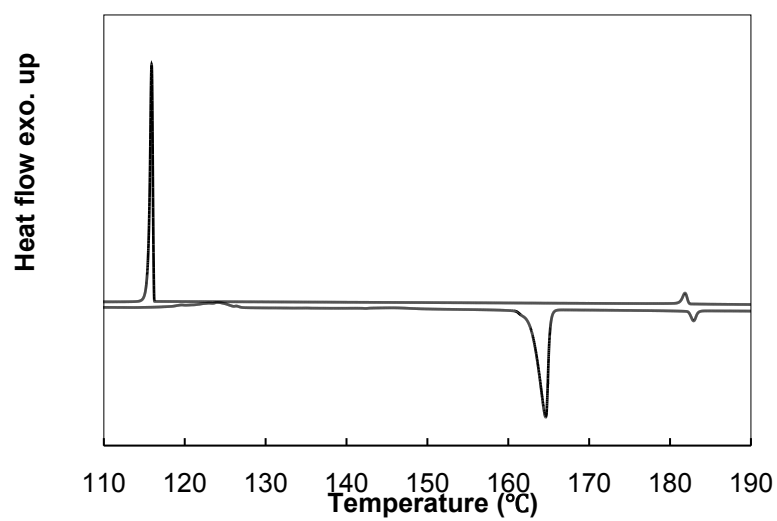


Fig. S10. DSC thermogram of 1OTO7OTO1.

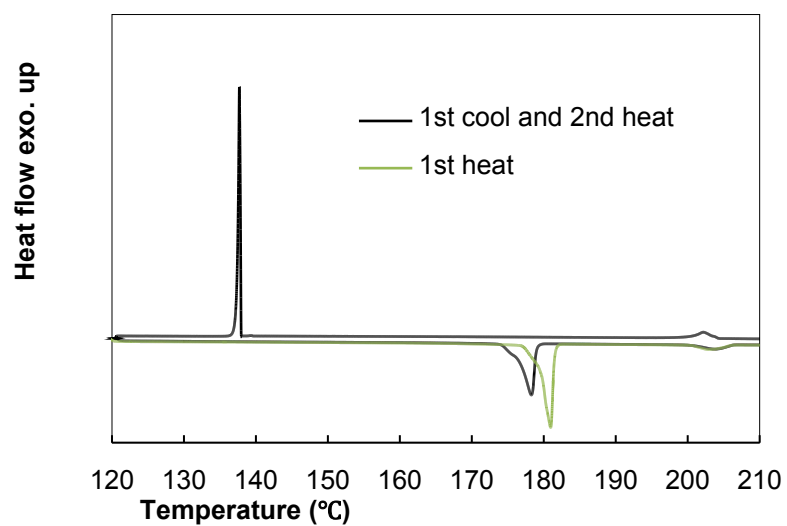


Fig. S11. DSC thermogram of 1OTO8OTO1. Different T_{CrN} values upon first and second heating were observed.

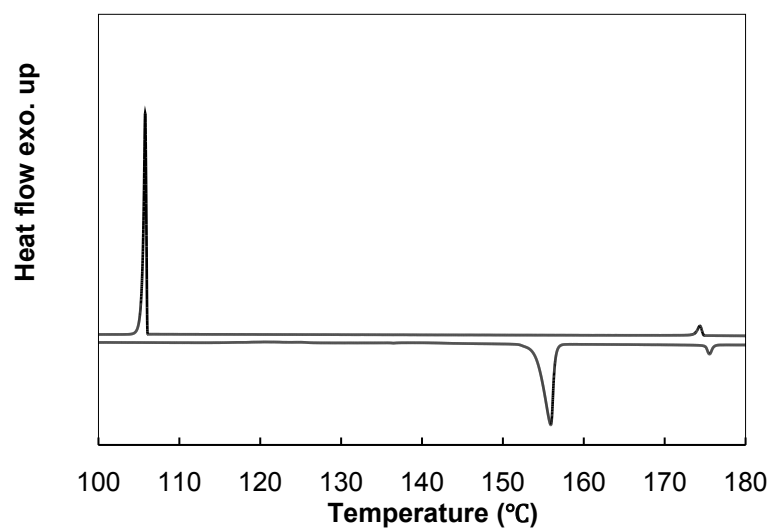


Fig. S12. DSC thermogram of 1OTO9OTO1.

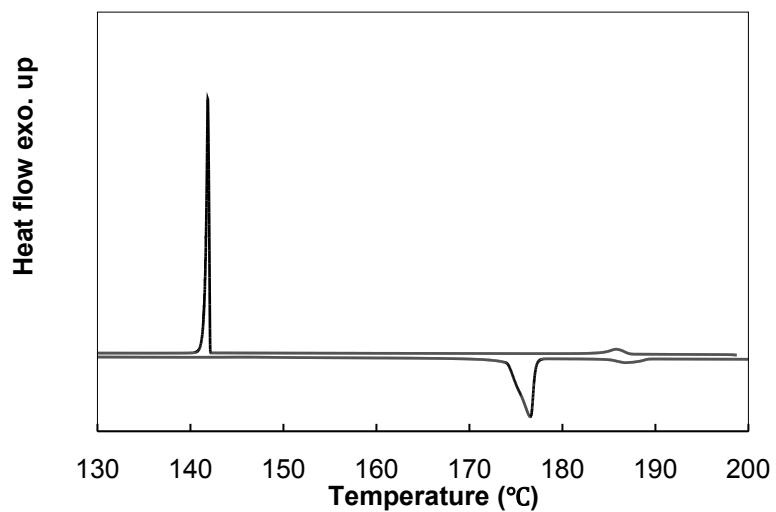


Fig. S13. DSC thermogram of 1OTO10OTO1.

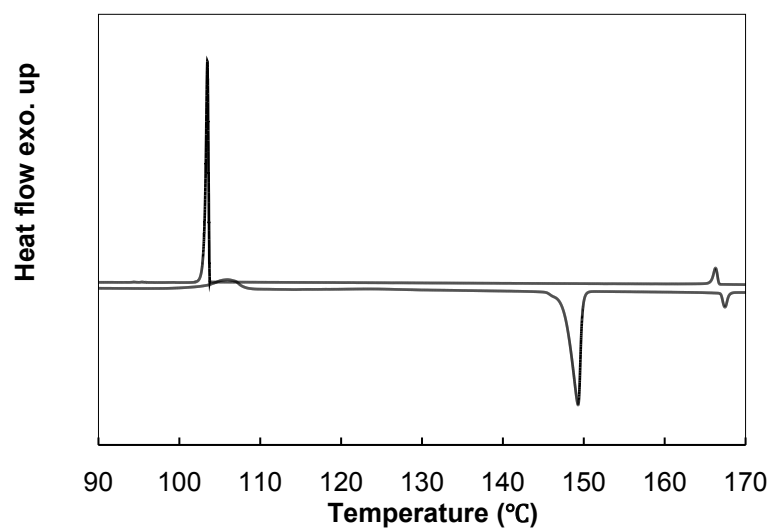


Fig. S14. DSC thermogram of 1OTO11OTO1.

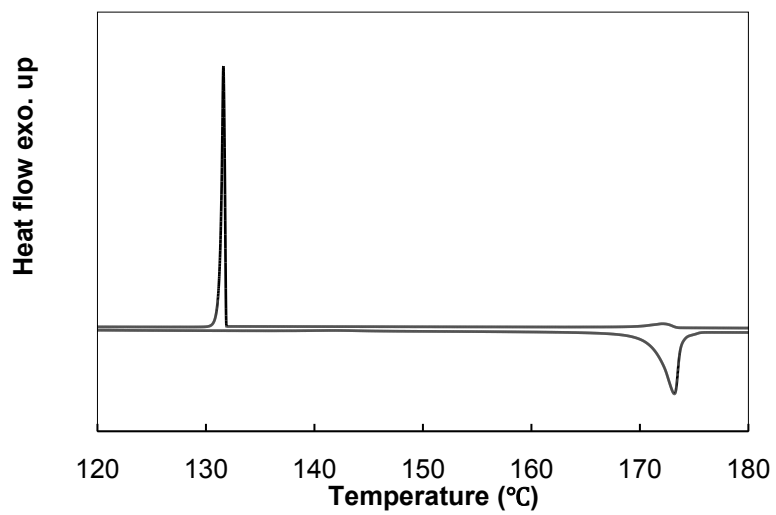


Fig. S15. DSC thermogram of 1OTO12OTO1.

Birefringence measurements

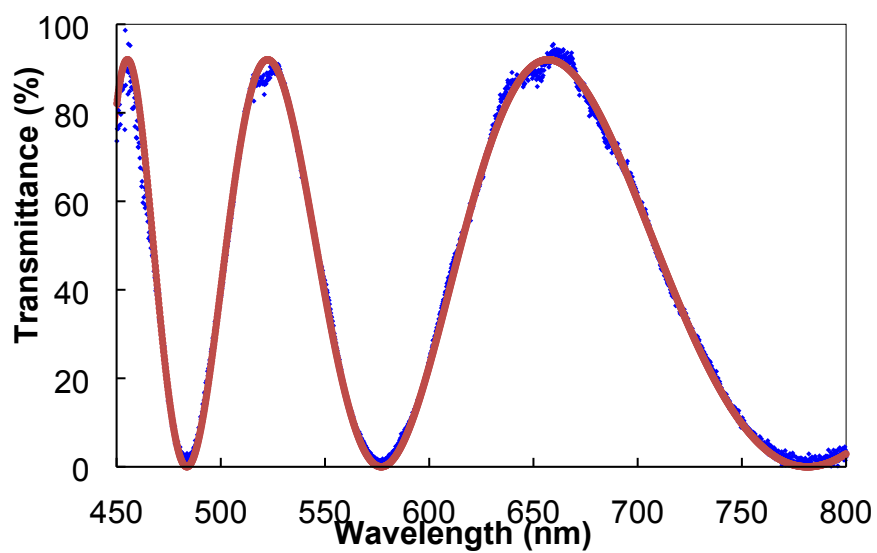


Fig. S16. The representative transmittance spectrum (blue dot) and fitting curve (red solid line) of a uniaxial specimen of 1OTO6OTO1 at 160 °C.

Table S1. Δn_0 and β values for 1OTOmOTO1.

m	Δn_0	β
5	0.4373	0.14
6	0.4374	0.11
7	0.3991	0.14
8	0.4692	0.14
9	0.3844	0.14
10	0.4485	0.13
11	0.3783	0.14
12	0.4181	0.13

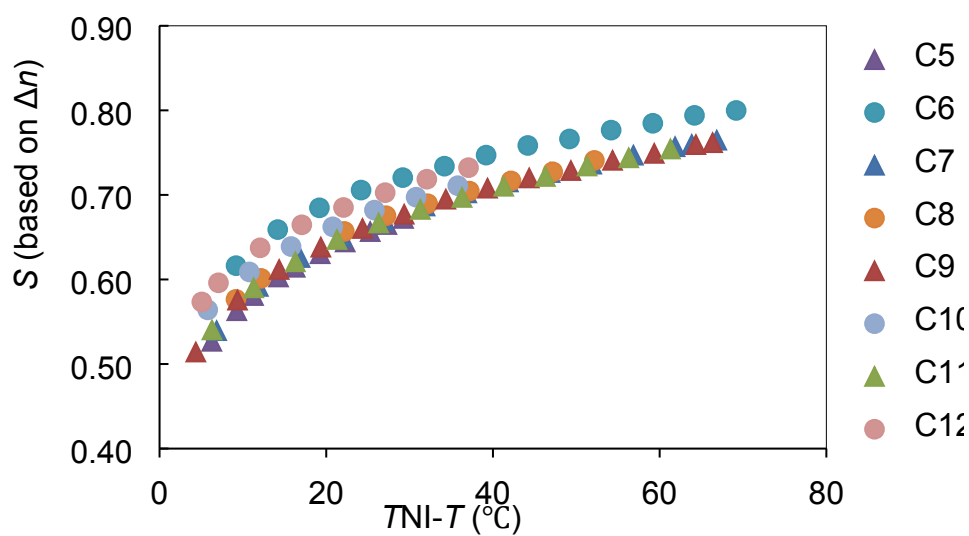


Fig. S17. Temperature dependence of the S values based on Haller's equation using Δn at 550 nm for 1OTOmOTO1.

UV-visible and fluorescent measurements

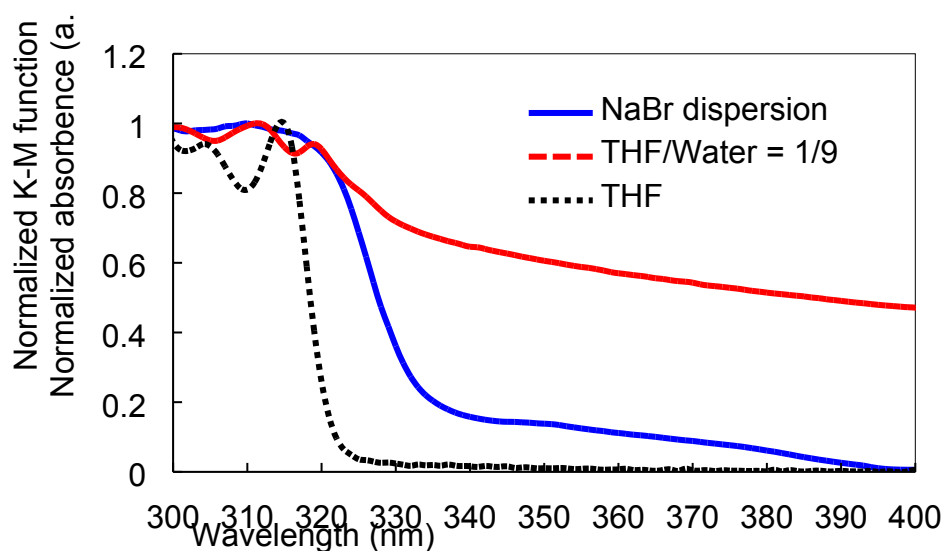


Fig. S18. UV-Vis and diffuse-reflectance spectra obtained from 1OTO10OTO1 in diluted solution, colloidal suspension (THF/Water = 1/9) and NaBr dispersion.

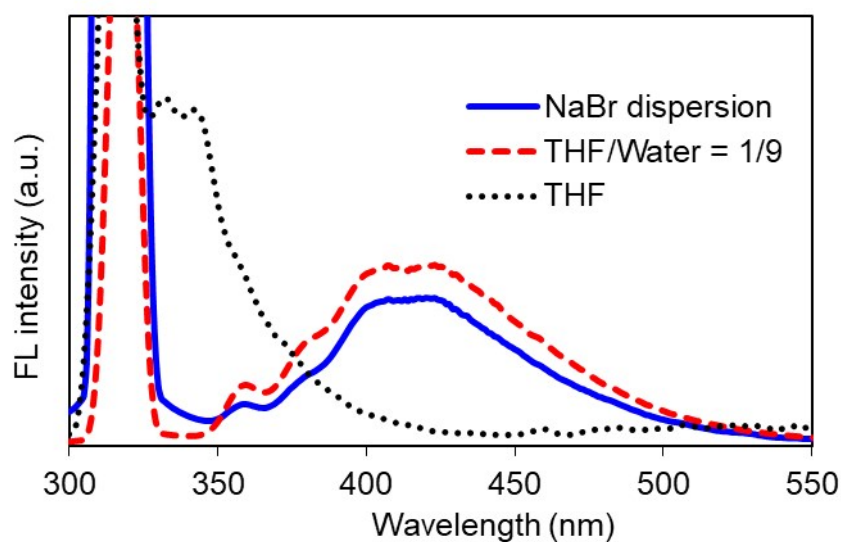


Fig. S19. Fluorescence (FL) spectra obtained from 1OTO10OTO1 in diluted solution (THF), colloidal suspension (THF/Water = 1/9) and NaBr dispersion.

Table S2. λ_{abs} , λ_{fl} and Φ_{fl} values in each condition for 1OTO10OTO1.

Condition	λ_{abs} (nm)	λ_{fl} (nm)	Φ_{fl} (%)
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Diluted solution ^a	295	304	315	333	343		≤ 0.01
Suspension ^b	300	311	300	360	405	422	0.23
NaBr dispersion ^c			310	359	407	420	0.34 ^d

^a in THF, ^b in THF/water = 1/9, ^c dispersed state in NaBr, and ^d from neat powder.