Supplementary Information

Thermally Reversible Full Color Selective Reflection in a Self-organized Helical Superstructure Enabled by a Bent-core Oligomesogen Exhibiting Twist-bend Nematic Phase

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1. Materials and Methods

All starting material, solvents and reagents were purchased from Sigma-Aldrich company and used without further purification. Column chromatography was carried out on silica gel (230-400 mesh). Analytical thin layer chromatography (TLC) was performed on commercially coated 60 mesh F254 glass plate. $^1$H NMR and $^{13}$C NMR spectra were recorded on a Bruker 400 spectrometer. Chemical shifts are reported in units (ppm) with the residual solvent (CDCl$_3$) peak as internal standard. Elemental analysis was performed by Roberston Microscopy Inc. Transition temperatures were taken at the maximum of transition peaks. The optical textures were captured by high-resolution CCD-equipped optical polarizing microscope (Leitz LABORLUX 12 POL, Germany). The reflective spectrum is detected by fiber-connected spectroscope (Ocean Opics USB 2000+). Freeze-fracture transmission electron microscopy (FF-TEM) experiment: The sample was heated to isotropic phase and cooled to 50°C slowly to get the N$_{hb}$ phase. The sample was then plunge frozen in liquid nitrogen and fractured at $T = -150$°C in a BalTec BAF060 freeze fracture apparatus. The fractured surface was replicated by the deposition of Pt/C (4 nm in thickness) at 45°.
followed by the deposition of a 20 nm C film. The replica was collected on carbon coated TEM grids and observed using a FEI Tecnai F20 TEM.


![Scheme S1. Synthetic route of twist-bend trimer 1](image)

3. Freeze-fracture transmission electron microscopy (FF-TEM) of the timer 1
Figure S1. FF-TEM image of N₆ trimer 1. The yellow dashed lines track the curved layers.

4. Reflection band-shifting of M₀₋₆ with the rising of temperature

Figure S2. Reflection band shift of the pure CLC M₀ (without trimer 1).
Figure S3. Reflection band shift of the CLC mixture $M_1$ with 2 wt% of trimer 1.

Figure S4. Reflection band shift of the CLC mixture $M_2$ with 6 wt% of trimer 1.
Figure S5. Reflection band shift of the CLC mixture $M_3$ with 8 wt% of trimer 1.

Figure S6. Reflection band shift of the CLC mixture $M_4$ with 10 wt% of trimer 1.

Figure S7. Reflection band shift of the CLC mixture $M_5$ with 12 wt% of trimer 1.
Figure S8. Correlation between temperature and wavelength shifting of mixtures M₁-₆. The starting temperature appearing the obvious band-shift for every sample is almost within the same temperature range (85–90 °C) as denoted by red-dashed ring.

5. Refractive index and birefringence of sample M₆ (nematic LC and trimer 1)

Figure S9. Correlation between the average refractive index of M₆ (nematic LC and 14 wt% trimer) and temperature.
Figure S10. Relationship between birefringence $\Delta n$ and ambient temperature in $M_b$ (nematic LC and 14 wt% trimer) and pure nematic LC, respectively.

6. Analysis for the relationship of $P_0/P - C_{\text{tri}}$

As shown in Figure 3a and b, the slope of the line is defined as a constant—helical twisted power ($HTP$) of the corresponding chiral dopant, i.e., $1/P = HTP \cdot C$. Herein, the concentration of chiral dopant should not be very large.

In the situation of high temperature, provided that the slope at the linear relationship is a constant $k$, thus,

$$\frac{P}{P_0} = k \cdot C_{\text{tri}}$$  (1)

where $P_0$ is the original pitch length without trimer dopant. Therefore, $P_0$ can be expressed by the helical twisted power of chiral dopant ($HTP_0$), and its concentration ($C_{\text{chiral}}$),

$$\frac{1}{P_0} = HTP_0 \cdot C_{\text{chiral}}$$  (2)

By combining Eqs. (1) and (2), the pitch length of a system with trimer dopant is

$$\frac{1}{P} = \frac{HTP_0}{k} \cdot \frac{C_{\text{chiral}}}{C_{\text{tri}}} = [HTP] \cdot [C]$$  (3)

$$[HTP] = \frac{HTP_0}{k} ; \quad [C] = \frac{C_{\text{chiral}}}{C_{\text{tri}}}$$  (4)

in which, $[HTP]$ and $[C]$ are defined respectively as the modulated helical twisted power and the modulated concentration of chiral dopant of the trimer doped system. The corresponding modulation parameters are $k$ and $C_{\text{tri}}$. Here, $k$ is determined by molecular interaction between
LCs and trimer molecules, and it is related to the molecular interaction. As shown in Figure 3b, for a fixed temperature \( k \) is a constant.

Equation (3) indicates that the helical pitch at a certain temperature of trimer-doped system can be expressed in the same form that a conventional chiral-doped system. The trimer \( 1 \) induces a weakened effect of helical twisted power, however such effect is only dependent on the aforementioned molecular interaction, \( \text{i.e., HTP-modulation parameter} \ k \), thus the modulated [HTP] is a constant at a certain temperature. From Figure 3b, as the temperature is increased, \( k \) gets larger and therefore the pitch length increases, thus explaining the observed red shift.

On the other hand, in the situation of low temperature, a non-linear relationship of \( P/P_0 \) and \( C_{\text{tri}} \) was shown in Fig. 3a, and can be expressed as,

\[
\frac{P}{P_0} = \frac{1}{a + b \cdot e^{cC_{\text{tri}}}}
\]

where \( a, b \) and \( c \) are fitting parameters.

Substituting Eq. (2) into Eq. (5), we obtain the expression of \( 1/P \),

\[
\frac{1}{P} = a \cdot \text{HTP}_0 \cdot C_{\text{chiral}} + b \cdot \text{HTP}_0 \cdot e^{cC_{\text{tri}}} \cdot C_{\text{chiral}}
\]

where \( a+b=1 \) (because \( P_0=P \) when \( C_{\text{tri}}=1 \)) and "\( e^{cC_{\text{tri}}} \)" is a non-linear factor which influences the HTP of the system. In Eq. (6), "\( c \)" is an interaction parameter determined by the molecular structure, solubility and the temperature. According to Eq. (6), when the temperature is invariable, with the increasing of trimer \( 1 \), the HTP of the system is strengthened. This HTP strengthening has been demonstrated in our experiment and the previous publications. In addition, as we mentioned in the manuscript, the bent-core having similar bent-angle and molecular length with the bent-core fragment of trimer \( 1 \) was doped into the same CLC host to repeat the same experiment, the similar chirality enhancement was observed, confirming the effect of bent-core fragment on the chirality enhancement, a fact that has been observed in other systems elsewhere.