Broad temperature range of cubic blue phase existed in simple binary mixture systems containing rodlike Schiff base mesogens with tolane moiety

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Electronic supplementary information (ESI)

Fig. S1 The DSC measurement of compounds (S)-OH-TI (blue line) and OH-TI (red line) on heating and cooling recycle.
**Fig. S2** Microphotographs for compound **OH-TI**

(a) N texture at 149.3°C; (b) N - SmC texture at 110.4°C; (c) SmC texture at 100.0°C; (d) CrG texture at 79.8°C; (e) CrH texture at 68.0°C.

**Fig S3.** Transition from mosaic texture of the soft crystal G to the soft crystal H of compound **OH-TI**, observed in the other area. (a) CrG texture at 78.6°C; (b) CrG-CrH texture at 75.8°C; (c) CrH texture at 70.0°C.
Fig. S4 The variable-temperature XRD measurements of compound OH-TI₇.
**Fig. S5** Microphotographs for compound (S)-H-TI$_7$

(a) BPII-BPI texture at 161.4°C; (b) BPI texture at 161.0°C; (c) N* texture at 160.9°C; (d) SmC* texture at 135.2°C; (e) SmC* texture in other area at 135.2°C; (f) CrG* texture at 126.6°C. This texture is of a mosaic kind, but retains schlieren characteristic from the smectic C phase; (g) CrH* texture at 99.8°C.

**Fig. S6** The DSC measurement of compounds (S)-H-TI (blue line) and H-TI (red line) on heating and cooling recycle.
Fig. S7 Microphotographs for compound H-TI

(a) N texture at 149.8°C; (b) N-SmC texture at 139.8°C; (c) SmC texture at 136.1°C; (d) CrG texture at 121.9°C; (e) CrH texture at 101.8°C.
Fig. S8 The comparison of BP temperature range for the different blending mixture systems in heating (red line) and cooling processes (blue line).
Fig. S9 Typical reflectance profiles of the higher-temperature phase (gray line) and the lower-temperature phase (black line) for the blending system mixture (a) OH-TI$_7$ + 40% S811 and (c) (S)-OH-TI$_7$ + 10% IOS(6OBA)$_2$. Temperature dependence of the Bragg reflection wavelength for the blending mixture consisting of OH-TI$_7$ + 40% S811 (b) and (S)-OH-TI$_7$ + 10% IOS(6OBA)$_2$ (d) during cooling process with a rate of 0.5 °C min$^{-1}$.

Fig. S10 Microphotographs for compound (S)-OH-TI blended with 40.0 wt% R811.
Measurements of helical pitch and helical twisting power of two chiral Schiff base mesogens and binary mixture system composed of 60 wt% racemic Schiff base and 40 wt% S811 by Cano’s Wedge method.

The helical pitch (p) was evaluated by measuring the distance (a) between Cano lines as follows: $p = 2a \tan \theta$, where $\theta$ is the angle of the wedge of the cell.

In this experiment, the cell’s $\tan \theta$ is 0.0196, the concentration of the chiral dopant c is 4%.
The DSC diagram, POM texture and XRD variable-temperature XRD of Schiff base mesogen OH-TI_{77}.

The DSC (Fig. S13) and POM pictures (Fig. S14) have indicated that Schiff base compound OH-TI_{77}, on cooling from its isotropic phase, displayed nematic Schlieren texture (N phase, Fig. S14a), straited texture below N-SmC transition (Fig. S14b), Schlieren texture with narrow dark four brushes (SmC phase, Fig. S14c), Schlieren texture with broader dark four-brushes (SmF phase, Fig. S14d), mosaic terrace-like relief with larger domains (the soft crystal CrG phase, Fig. S14e), mosaic texture with small platelet area that are cross-hatched by grainings (the soft crystal CrH phase, Fig. S14f) and two crystal phase (Fig. S14g and Fig. S14h).

![DSC diagram](image.png)

**Fig. S13** The DSC measurement of compounds OH-TI_{77} on heating (red line) and cooling recycle (blue line).
Fig. S14 Microphotographs of compound \textbf{OH-TI$_{77}$} observed under the POM: (a) N texture at 210.0°C; (b) N - SmC transition texture at 181.6°C; (c) SmC texture at 130.0°C; (d) SmF texture at 120.0°C; (e) CrG texture at 112.0°C; (f) CrH texture at 100.0°C; (g) Cr$_1$ texture at 87.8°C; (h) Cr$_2$ texture at 74.2°C.
Fig. S15 The variable-temperature XRD measurements of compound OH-TI\textsubscript{77}. 

(a) OH-TI\textsubscript{77}, T = 150°C

(b) OH-TI\textsubscript{77}, T = 112°C

(c) OH-TI\textsubscript{77}, T = 100°C

(d) OH-TI\textsubscript{77}, T = 88°C

(e) OH-TI\textsubscript{77}, T = RT

CrH
Monoclinic
- \(a = 33.43(1) \text{ Å}\)
- \(b = 4.628(2) \text{ Å}\)
- \(c = 20.76(1) \text{ Å}\)
- \(\beta = 92.75(3)^\circ\)

Cr\textsubscript{1}
Hexagonal
- \(q_1 = 0.2387 (\text{Å})\)
- \(q_2 = 0.4613 (\text{Å})\)
- \(q_3 = 1.4139 (\text{Å})\)
- \(a = 5.13 (\text{Å})\)
- \(c = 27.24 (\text{Å})\)

Cr\textsubscript{2}
Monoclinic
- \(a = 33.43(1) \text{ Å}\)
- \(b = 4.628(2) \text{ Å}\)
- \(c = 20.76(1) \text{ Å}\)
- \(\beta = 92.75(3)^\circ\)
Fig. S16. HOMO and LUMO of Schiff base compound (a), Salicylaldimine compound (b) and compound OH-TI$_{77}$ (c). The simulation exchange functional and basis set are CAM-B3LYP and 6-311G(d, p), respectively. The isosurface is drawn at value of 0.02.
Table S1. A comparison table with different basis sets and exchange functionals on the calculated dipole moment in Schiff base compound, Salicylaldimine compound and compound OH-TI$_{77}$.

<table>
<thead>
<tr>
<th>Exchange functional</th>
<th>Basis set</th>
<th>Dipole Moment (Debye)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Schiff base</td>
<td>Salicylaldimine</td>
</tr>
<tr>
<td>CAM-B3LYP</td>
<td>6-31G(d,p)</td>
<td>1.8072</td>
</tr>
<tr>
<td></td>
<td>def2-tzvp</td>
<td>1.9057</td>
</tr>
<tr>
<td></td>
<td>6-31G(d)</td>
<td>1.8032</td>
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<tr>
<td></td>
<td>6-31+G(d)</td>
<td>1.9425</td>
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<tr>
<td>oB97X</td>
<td>6-31G(d,p)</td>
<td>1.6789</td>
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<tr>
<td></td>
<td>6-31G(d)</td>
<td>1.6739</td>
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<tr>
<td></td>
<td>6-31+G(d)</td>
<td>2.1211</td>
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Table S2. DFT calculated HOMO, LUMO, energy gap, dipole moment components, $\mu_x$, $\mu_y$, $\mu_z$ and modulus ($\mu$) for Schiff base compound, Salicylaldimine compound and compound OH-TI$_{77}$.

<table>
<thead>
<tr>
<th>Exchange functional and Basis set</th>
<th>Compound</th>
<th>Energy (eV)</th>
<th>Dipole moment ($\mu$ in Debye)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CAM-B3LYP 6-311G(d,p)</td>
<td>Schiff base</td>
<td>-6.697</td>
<td>-1.058</td>
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<tr>
<td></td>
<td>Salicylaldimine</td>
<td>-6.736</td>
<td>0.543</td>
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<tr>
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<td>OH-TI$_{77}$</td>
<td>-6.766</td>
<td>0.296</td>
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<tr>
<td>oB97X 6-311G(d,p)</td>
<td>Schiff base</td>
<td>-7.641</td>
<td>-0.937</td>
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<tr>
<td></td>
<td>Salicylaldimine</td>
<td>-7.689</td>
<td>0.478</td>
</tr>
<tr>
<td></td>
<td>OH-TI$_{77}$</td>
<td>-7.701</td>
<td>0.286</td>
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</tbody>
</table>

Table S3. DFT calculated principal polarizability components ($\alpha_{XX}$, $\alpha_{YY}$, $\alpha_{ZZ}$), isotropic component $\alpha^{iso} = (\alpha_{XX}+\alpha_{YY}+\alpha_{ZZ})/3$, polarizability anisotropy $\Delta \alpha = [\alpha_{XX}-(\alpha_{YY}+\alpha_{ZZ})]/2$ and asymmetry parameter $\eta_a = [(\alpha_{YY}-\alpha_{ZZ})/(\alpha_{XX}-\alpha^{iso})]$, relative to the molecular polarizability tensor $\alpha$.

<table>
<thead>
<tr>
<th>Exchange functional and Basis set</th>
<th>Compound</th>
<th>$\alpha_{XX}$</th>
<th>$\alpha_{YY}$</th>
<th>$\alpha_{ZZ}$</th>
<th>$\alpha^{iso}$</th>
<th>$\Delta \alpha$</th>
<th>$\eta_a$</th>
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<tbody>
<tr>
<td>CAM-B3LYP 6-311G(d,p)</td>
<td>Schiff base</td>
<td>874.25</td>
<td>374.57</td>
<td>256.32</td>
<td>501.71</td>
<td>558.81</td>
<td>0.31742</td>
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<td></td>
<td>Salicylaldimine</td>
<td>892.29</td>
<td>380.81</td>
<td>256.42</td>
<td>509.84</td>
<td>573.68</td>
<td>0.32525</td>
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<tr>
<td></td>
<td>OH-TI$_{77}$</td>
<td>897.57</td>
<td>353.14</td>
<td>246.43</td>
<td>499.05</td>
<td>597.79</td>
<td>0.26777</td>
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<tr>
<td>oB97X 6-311G(d,p)</td>
<td>Schiff base</td>
<td>818.70</td>
<td>373.20</td>
<td>261.67</td>
<td>484.53</td>
<td>501.27</td>
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<td>Salicylaldimine</td>
<td>837.45</td>
<td>376.35</td>
<td>264.11</td>
<td>492.64</td>
<td>517.22</td>
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<td>OH-TI$_{77}$</td>
<td>846.19</td>
<td>351.98</td>
<td>249.84</td>
<td>482.67</td>
<td>545.28</td>
<td>0.28098</td>
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References: