**Supporting Information**

**Room-temperature AIE ionic liquid crystals based on diphenylacrylonitrile-imidazole salts**

Hongyu Guo,a,b Qi Yu,a Yuzhi Xiong,a,b and Fafu Yang*a,c

a. College of Chemistry and Materials Science, Fujian Normal University, Fuzhou 350007, P. R. China; Email: yangfafu@fjnu.edu.cn. b. Fujian Key Laboratory of Polymer Materials, Fuzhou 350007, P. R. China. c. Fujian provincial Key Laboratory of Advanced Materials Oriented Chemical Engineering, Fuzhou 350007, P. R. China.

1. General

All chemical reagents including organic and inorganic compounds were obtained by Aladdin Reagent Co., Ltd. and used directly. Pre-coated glass plates were used for TLC detection. Column chromatography was performed on using silica gel (200-300 mesh). Bruker-ARX 400 instrument was used for measuring the NMR spectra with tetramethylsilane (TMS) as internal standard. Bruker mass spectrometer was applied for MS spectral analysis. UV-Vis spectra were recorded on Varian UV-Vis spectrometer. Edinburgh Instruments FS5 spectrometer was used for examining fluorescence spectra. The fluorescence absolute ΦF values were investigated on an Edinburgh Instruments FLS920 Fluorescence Spectrometer bearing a 6-inch integrating sphere. Compounds 3 and 4 were prepared according to the published procedure (The influence of multiple alkyl chains on mesomorphic and photophysical properties of diphenylacrylonitrile liquid crystals, Liangbin Lin; Wenwei Qin; Bifeng Cheng; Hongyu Guo; Fafu Yang, Liquid Crystals, 2020,10.1080/02678292.2019.1692931).
2. The synthetic process and characteristic spectra.

2.1 Synthesis of compounds 5 and 6

A mixture of compound 3 or 4 (2.0 mmol), bromochloropropane (0.37 g, 2.0 mmol) and K₂CO₃ (1.4 g, 10 mmol) in 45 mL of dry MeCN was refluxed at 83 °C for 12 h. The reaction was monitored by TLC analysis. After reaction, 40 mL of HCl solution (1M) and 45 mL of CH₂Cl₂ were poured in the reaction system. Then the organic layer was separated and concentrated under reduced pressure. The residue was further purified by column
chromatography with CH$_2$Cl$_2$/hexane (3:7, V/V) as eluent. Compounds 5 and 6 were obtained as yellow solid in yields of 70% and 68%, respectively.

Compound 5: $^1$H NMR (400 MHz, CDCl$_3$) $\delta$: 7.84(d, $J = 8.0$ Hz, 2H, ArH), 7.57(d, $J = 8.0$ Hz, 2H, ArH), 7.35(s, 1H, CH=C), 6.95(d, $J = 8.0$ Hz, 4H, ArH), 4.14( $t$, $J = 6.0$ Hz, 2H, ClCH$_2$), 4.01 (t, $J = 6.0$ Hz, 2H, OCH$_2$). 3.76(t, $J = 6.0$ Hz, 2H, OCH$_2$), 2.24 (m, 2H, OCH$_2$CH$_2$), 1.78-1.82(t, 2H, OCH$_2$CH$_2$), 1.27-1.46(m, 18H, CH$_2$), 0.86(t, $J = 6.0$ Hz, 3H, CH$_3$).

Compound 6: $^1$H NMR (400 MHz, CDCl$_3$) $\delta$: 7.62(s, 1H, ArH), 7.57 (d, $J = 8.0$ Hz, 2H, ArH), 7.32(bs, 2H, ArH and CH=C), 6.95 (d, $J = 8.0$ Hz, 2H, ArH), 6.90 (d, $J = 8.0$ Hz, 1H, ArH), 4.16(t, $J = 6.0$ Hz, 2H, ClCH$_2$), 4.04-4.10(m, 4H, OCH$_2$), 3.76(t, $J = 6.0$ Hz, 2H, OCH$_2$), 0.86-2.29 (m, 48H, CH$_2$ and CH$_3$).

2.2 Synthesis of compounds 1C-I and 2C-I

The mixture of compound 5 or 6 (0.5 mmol), 1-methylimidazole (0.04 g, 0.5 mmol) and KI (0.17 g, 1 mmol) was refluxed in dry MeCN at 83 $^\circ$C for 4 h. The reaction was monitored by TLC analysis. After reaction, the solvent was distilled under reduced pressure. The residue was purified by column chromatography with CH$_2$Cl$_2$/MeOH (9:1, V/V) as eluent. Compounds 1C-I and 2C-I were obtained as yellow viscous substance in yields of 65% and 63%, respectively.

Compound 1C-I: $^1$H NMR (400 MHz, CDCl$_3$) $\delta$: 9.88 (s, 1H, ArH), 7.80 (d, $J = 8.0$ Hz, 2H, ArH), 7.51 (d, $J = 8.0$ Hz, 2H, ArH), 7.47 (s, 1H, ArH), 7.43(s, 1H, ArH), 7.32(s, 1H, CH=C), 6.91(d, $J = 8.0$ Hz, 4H, ArH), 4.59(t, $J = 6.0$ Hz, 2H, NCH$_2$), 4.09(t, $J = 6.0$ Hz, 2H, OCH$_2$), 4.04 (s, 3H, NCH$_3$) 3.96(t, $J = 6.0$ Hz, 2H, OCH$_2$), 1.47-2.48(m, 22H, CH$_2$), 0.86 (t, $J = 6.0$ Hz,3H,CH$_3$). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$: 160.78, 158.59, 140.29, 137.07, 130.85, 127.64, 127.02, 126.28, 123.67, 122.58, 118.76, 114.99, 114.74, 107.32, 68.19, 64.59, 47.19, 36.91, 31.78, 29.81, 29.63, 29.43, 29.01, 26.00, 22.67, 14.11. MALDI-TOF-MS (C$_{34}$H$_{46}$N$_3$O$_2$I) Calcd. For $m/z$ = 528.359, found: 528.502. Anal. Calcd for C$_{34}$H$_{46}$N$_3$O$_2$I: C, 62.28; H, 7.07; N, 6.41. Found: C, 62.24; H, 7.01; N, 6.35.

Compound 2C-I: $^1$H NMR (400 MHz, CDCl$_3$) $\delta$: 10.06(s, 1H, ArH), 7.60(s, 1H,ArH), 7.55(d, $J = 8.0$ Hz, 2H, ArH), 7.32-7.38(m, 4H,ArH and CH=C), 6.93 (d, $J= 8.0$ Hz, 2H, ArH), 6.89(d, $J = 8.0$ Hz, 1H, ArH), 4.61( t, $J = 6.0$ Hz, 2H,NCH$_2$), 4.06-4.14(m, 9H, OCH$_2$ and
CH₃), 0.86-2.52(m, 48H, CH₂ and CH₃). ¹³C NMR (101 MHz, CDCl₃) δ: 158.52, 151.22, 148.91, 140.74, 137.08, 127.94, 127.16, 126.67, 123.99, 123.50, 122.48, 118.91, 115.02, 112.87, 107.48, 69.32, 69.10, 64.38, 47.39, 37.24, 31.91, 29.64, 29.36, 29.22, 29.00, 26.07, 26.00, 22.68, 14.10. MALDI-TOF-MS (C₄₆H₇₀N₃O₃) Calcd. for m/z = 712.542. Found: 712.572. Anal. Calcd for C₄₆H₇₀N₃O₃I: C, 65.78; H, 8.40; N, 5.00. Found: C, 65.72; H, 8.44; N, 4.96.

2.3 Synthesis of compounds 1C-T, 2C-T, 1C-P and 2C-P

The mixture of compound 1C-I or 2C-I (0.5 mmol) and sodium trifluoroacetate or sodium p-toluenesulfonate (2.5 mmol) was stirred in MeOH/CH₂Cl₂ (2:8) at 65°C for 4h. After reaction, the solvent was evaporated under reduced pressure. The obtained yellow sticky product was washed by distilled water and then was dried under vacuum to afford sticky compounds 1C-T, 2C-T, 1C-P and 2C-P in yields of 75%, 78%, 80% and 76%, respectively.

Compound 1C-T: ¹H NMR (400 MHz, CDCl₃) δ: 9.64 (s, 1H, ArH), 7.76 (d, J = 8.0 Hz, 2H, ArH), 7.45 (d, J = 8.0 Hz, 2H, ArH), 7.38-7.44 (m, 3H, ArH), 6.87(d, J = 8.0 Hz, 2H, ArH), 6.83(d, J = 8.0 Hz, 2H, ArH), 4.41(bs, 2H, NCH₂), 3.86-3.96(m, 7H, OCH₂ and NCH₃), 1.25-2.33(m, 22H, CH₂), 0.84 (t, J = 6.0 Hz,3H,CH₃). ¹³C NMR (101 MHz, CDCl₃) δ: 160.82, 158.63, 140.31, 137.62, 131.55, 130.93, 130.18, 127.72, 126.99, 126.30, 123.53, 122.48, 118.74, 114.83, 114.47, 107.44, 68.19, 64.27, 47.00, 36.12, 31.90, 31.58, 29.58, 29.34, 29.16, 25.99, 22.59, 13.92. MALDI-TOF-MS(C₃₄H₄₆N₃O₂) Calcd. for m/z = 528.359. Found: 528.583. Anal. Calcd for C₃₆H₄₆N₃O₄F₃: C, 67.37; H, 7.22; N, 6.55. Found: C, 67.32; H, 7.25; N, 6.50.

Compound 2C-T: ¹H NMR (400 MHz, CDCl₃) δ: 9.79 (s, 1H, ArH), 7.76 (d, J = 8.0 Hz, 2H, ArH), 6.90(m, 3H, ArH), 4.53(bs, 2H, NCH₂), 3.99-4.06(m, 9H, OCH₂ and NCH₃), 2.42(bs, 2H, CH₂), 1.84(bs, 4H, CH₂), 1.27(bs, 36H, CH₃), 0.89(bs, 6H, CH₃). ¹³C NMR (101 MHz, CDCl₃) δ: 158.57, 151.19, 149.05, 140.78, 137.67, 130.48, 127.92, 127.10, 126.65, 126.07, 123.93, 123.47, 122.46, 118.83, 114.90, 113.24, 112.82, 107.45, 69.28, 69.06, 64.29, 47.18, 36.56, 31.91, 29.64, 29.36, 29.10, 25.93, 22.67, 14.10. MALDI-TOF-MS (C₄₆H₇₀N₃O₃) Calcd. for m/z = 712.542. Found: 712.376. Anal. Calcd for C₄₆H₇₀N₃O₃F₃: C, 69.79; H, 8.54; N, 5.09. Found: C, 69.73; H, 8.58; N, 5.02.

Compound 1C-P: ¹H NMR (400 MHz, CDCl₃) δ: 9.73 (s, 1H, ArH), 7.78 (d, J = 8.0 Hz, 2H, ArH), 6.94-7.74 (m, 29H, ArH), 3.99-4.06(m, 7H, OCH₂ and NCH₃), 1.27(bs, 36H, CH₃), 0.89(bs, 6H, CH₃). ¹³C NMR (101 MHz, CDCl₃) δ: 158.57, 151.19, 149.05, 140.78, 137.67, 130.48, 127.92, 127.10, 126.65, 126.07, 123.93, 123.47, 122.46, 118.83, 114.90, 113.24, 112.82, 107.45, 69.28, 69.06, 64.29, 47.18, 36.56, 31.91, 29.64, 29.36, 29.10, 25.93, 22.67, 14.10. MALDI-TOF-MS (C₄₆H₇₀N₃O₃) Calcd. for m/z = 712.542. Found: 712.376. Anal. Calcd for C₄₆H₇₀N₃O₃F₃: C, 69.79; H, 8.54; N, 5.09. Found: C, 69.73; H, 8.58; N, 5.02.
2H, ArH), 7.44-7.49 (m, 4H, ArH), 7.31 (s, 1H, CH=C), 7.22 (d, J= 8.0 Hz, 2H, ArH), 7.07 (d, J= 8.0 Hz, 2H, ArH), 6.87-6.90 (m, 4H, ArH), 4.53 (t, J= 8.0 Hz, 2H, NCH₂), 4.04 (t, J= 8.0 Hz, 2H, OCH₂), 3.99 (s, 3H, NCH₃), 3.94 (t, J= 8.0 Hz, 2H, OCH₂), 3.99 (s, 3H, NCH₃), 3.94 (t, J= 8.0 Hz, 2H, OCH₂), 2.23-2.48 (m, 5H, CH₂ and CH₃), 1.21-1.78 (m, 20H, CH₂), 0.84 (t, 3H, CH₃). ¹³C NMR (101 MHz, CDCl₃) δ: 160.84, 158.56, 143.31, 140.61, 137.05, 131.58, 130.98, 130.26, 127.90, 127.12, 126.42, 125.77, 123.58, 122.71, 118.83, 115.11, 114.81, 107.49, 68.33, 64.42, 53.37, 47.49, 37.11, 32.07, 29.60, 29.34, 25.97, 22.67, 14.20. MALDI-TOF-MS (C₃₄H₄₆N₃O₂) Calcd. For m/z = 528.359, found: 528.257. Anal. Calcd for C₄₁H₅₃N₃O₅S: C, 70.35; H, 7.63; N, 6.00. Found: C, 70.32; H, 7.68; N, 5.94.

Compound 2C-P: ¹H NMR (400 MHz, CDCl₃) δ: 9.40 (s, 1H, ArH), 7.74 (bs, 2H, ArH), 7.61 (s, 1H, ArH), 7.47 (bs, 2H, ArH), 7.29 (bs, 4H, CH=C and ArH), 7.12 (bs, 2H, ArH), 6.83 (bs, 3H, ArH), 4.38 (bs, 2H, NCH₂), 3.84-4.12 (m, 9H, OCH₂ and NCH₃), 2.28 (bs, 5H, CH₂ and CH₃), 1.84 (bs, 4H, CH₂), 1.28 (bs, 36H, CH₂), 0.89 (t, 6H, CH₃). ¹³C NMR (101 MHz, CDCl₃) δ: 158.66, 151.15, 148.96, 143.24, 140.66, 139.75, 137.54, 128.83, 127.77, 127.05, 126.69, 125.81, 123.97, 123.47, 122.33, 118.83, 114.94, 112.93, 112.77, 107.52, 69.26, 68.96, 64.43, 53.47, 47.01, 36.40, 31.94, 29.67, 29.46, 29.39, 29.17, 26.10, 22.70, 21.27, 14.13. MALDI-TOF-MS (C₄₆H₇₀N₃O₃) Calcd. for m/z = 712.542. Found: 712.430. Anal. Calcd for C₅₃H₇₇N₃O₆S: C, 71.99; H, 8.78; N, 4.75. Found: C, 71.94; H, 8.76; N, 4.70.
Figure S1. The $^1$H NMR spectrum of compound 5

Figure S2. The $^1$H NMR spectrum of compound 6
Figure S3. The $^1$H NMR spectrum of compound 1C-I

Figure S4. The $^{13}$C NMR spectrum of compound 1C-I
Figure S5. The MALDI-TOF-MS spectrum of compound 1C-I

Figure S6. The $^1$H NMR spectrum of compound 2C-I
Figure S7. The $^{13}$C NMR spectrum of compound 2C-I

Figure S8. The MALDI-TOF-MS spectrum of compound 2C-I
Figure S9. The $^1$H NMR spectrum of compound 1C-T

Figure S10. The $^{13}$C NMR spectrum of compound 1C-T
Figure S11. The MALDI-TOF-MS spectrum of compound 1C-T

Figure S12. The $^1$H NMR spectrum of compound 2C-T
Figure S13. The $^{13}$C NMR spectrum of compound 2C-T

Figure S14. The MALDI-TOF-MS spectrum of compound 2C-T
Figure S15. The \(^1\)H NMR spectrum of compound 1C-P

Figure S16. The \(^{13}\)C NMR spectrum of compound 1C-P
Figure S17. The MALDI-TOF-MS spectrum of compound 1C-P

Figure S18. The $^1$H NMR spectrum of compound 2C-P
Figure S19. The $^{13}$C NMR spectrum of compound 2C-P

Figure S20. The MALDI-TOF-MS spectrum of compound 2C-P
Figure S21 The XRD pattern of 1C-I

Figure S22 The XRD pattern of 1C-T
Figure S23 The XRD pattern of 1C-P

Figure S24 The XRD pattern of 2C-I
Figure S25 The XRD pattern of 2C-T

Figure S26 The XRD pattern of 2C-P
Figure S27 The UV-vis absorption spectra of 1C-I, 1C-T, 1C-P, 2C-I, 2C-T and 2C-P (1.0×10⁻⁵ M in THF solution, each)

Figure S28 Fluorescence emission spectra of 1C-I in THF-H₂O solution (1×10⁻⁵ M, λₑₓ = 350 nm). Inset: Fluorescence photos of 1C-I at 0% and 95% H₂O fractions.
**Figure S29** Fluorescence emission spectra of 1C-T in THF-H$_2$O solution (1×10$^{-5}$ M, $\lambda_{ex}$ = 350 nm). Inset: Fluorescence photos of 1C-T at 0% and 95% H$_2$O fractions.

**Figure S30** Fluorescence emission spectra of 1C-P in THF-H$_2$O solution (1×10$^{-5}$ M, $\lambda_{ex}$ = 350 nm). Inset: Fluorescence photos of 1C-P at 0% and 95% H$_2$O fractions.
**Figure S31** Fluorescence emission spectra of 2C-I in THF-H₂O solution (1×10⁻⁵ M, λₑₓ = 350 nm). Inset: Fluorescence photos of 1C-I at 0% and 95% H₂O fractions.

**Figure S32** Fluorescence emission spectra of 2C-T in THF-H₂O solution (1×10⁻⁵ M, λₑₓ = 350 nm). Inset: Fluorescence photos of 1C-T at 0% and 95% H₂O fractions.
**Figure S33** Fluorescence emission spectra of 2C-P in THF-H$_2$O solution (1×10$^{-5}$ M, $\lambda_{ex}$ = 350 nm). Inset: Fluorescence photos of 1C-P at 0% and 95% H$_2$O fractions.

**Figure S34** Fluorescence spectra of 1C-I, 1C-T, 1C-P, 2C-I, 2C-T and 2C-P in solid films ($\lambda_{ex}$ = 350 nm).
Figure S35  CVs of 1C-I, 1C-T and 1C-P (1 mM) in 5% ethanol (at a scan rate of 50 mV s\(^{-1}\))

Figure S36  CVs of 2C-I, 2C-T and 2C-P (1 mM) in 5% ethanol (at a scan rate of 50 mV s\(^{-1}\))
**Figure S37** CVs of 1C-I (1 mM) in 5% ethanol at different scan rates

**Figure S38** CVs of 1C-T (1 mM) in 5% ethanol at different scan rates
**Figure S39** CVs of 1C-P (1 mM) in 5% ethanol at different scan rates

**Figure S40** CVs of 2C-I (1 mM) in 5% ethanol at different scan rates
**Figure S41** CVs of 2C-T (1 mM) in 5% ethanol at different scan rates

**Figure S42** CVs of 2C-P (1 mM) in 5% ethanol at different scan rates

**Table S1** Transition temperatures (°C) and enthalpies (kJ·mol⁻¹) of Novel AIE ILCs
<table>
<thead>
<tr>
<th>sample</th>
<th>Phase transition[a]</th>
<th>Heating scan $T(\Delta H)$</th>
<th>Cooling scan $T(\Delta H)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1C-I</td>
<td>Cr-SmA (SmA-Cr)</td>
<td>41.0(14.8)</td>
<td>146.6(4.4)</td>
</tr>
<tr>
<td></td>
<td>SmA-Iso(Iso-SmA)</td>
<td>41.5(15.4)</td>
<td>135.6(4.1)</td>
</tr>
<tr>
<td>1C-T</td>
<td>Cr-SmA (SmA-Cr)</td>
<td>50.8(13.9)</td>
<td>162.2(3.6)</td>
</tr>
<tr>
<td></td>
<td>SmA-Iso(Iso-SmA)</td>
<td>50.6(12.7)</td>
<td>160.4(4.8)</td>
</tr>
<tr>
<td>1C-P</td>
<td>Cr-SmA (SmA-Cr)</td>
<td>39.8(17.2)</td>
<td>147.2(4.8)</td>
</tr>
<tr>
<td></td>
<td>SmA-Iso(Iso-SmA)</td>
<td>37.0(15.8)</td>
<td>139.2(4.0)</td>
</tr>
<tr>
<td>2C-I</td>
<td>Cr-Col$<em>h$ (Col$</em>{h}$-Cr)</td>
<td>34.6(19.6)</td>
<td>163.1(2.8)</td>
</tr>
<tr>
<td></td>
<td>Col$<em>{h}$-Iso(Col$</em>{h}$)</td>
<td>19.8(18.2)</td>
<td>147.3(2.1)</td>
</tr>
<tr>
<td>2C-T</td>
<td>Cr-Col$<em>{h}$ (Col$</em>{h}$-Cr)</td>
<td>47.5(17.4)</td>
<td>205.6(2.6)</td>
</tr>
<tr>
<td></td>
<td>Col$<em>{h}$-Iso(Col$</em>{h}$)</td>
<td>25.6(16.3)</td>
<td>195.4(2.4)</td>
</tr>
<tr>
<td>2C-P</td>
<td>Cr-Col$<em>{h}$ (Col$</em>{h}$-Cr)</td>
<td>29.0(17.2)</td>
<td>181.6(3.4)</td>
</tr>
<tr>
<td></td>
<td>Col$<em>{h}$-Iso(Col$</em>{h}$)</td>
<td>16.1(16.9)</td>
<td>175.1(2.9)</td>
</tr>
</tbody>
</table>

[a] Cr = crystalline, SmA = SmA mesophase, Col$_h$ = hexagonal columnar mesophase, Iso = isotropic

**Figure S43** Fluorescence emission spectra of 1C-T in THF-petroleum ether solution ($1 \times 10^{-5}$ M, $\lambda_{ex} = 350$ nm).