Electronic Supplementary Material (ESI) for Faraday Discussions.

SUPPORTING INFORMATION

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S1. The synthetic route of (2Z, 2'Z)-3,3'-(1,4-phenylene)bis(2-(naphthalen-2-yl) acrylonitrile (PBNA)

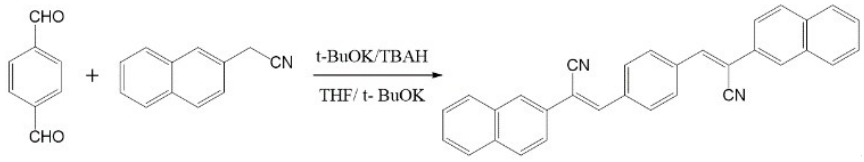

Figure 1. The synthetic scheme of PBNA compound

The compound PBNA was synthesized by a typical Knoevenagel condensation, as shown in Figure 1. All chemicals were purchased commercially and used without further purification. 2-Naphthylacetonitrile (334.42 mg, 2 mmol) and terephthalaldehyde (134.13 mg, 1 mmol) were dissolved in tertiary butanol (10 mL) and tetrahydrofuran, stirred at 50 °C for 30 min under a nitrogen atmosphere. Then, potassium tertbutoxide (1mol/L, 0.25 mL) and tetrabutylammonium hydroxide (TBAH) (1 mol/L, 0.25 mL) were added into the mixture and kept stirring for 20 min. After adding a drop of acetic acid, the resulting precipitate was poured into the methanol acidized and then filtered and purified by dichloromethane. Solid powder PBNA (326 mg) was obtained with the yield of 75 %. The MALDI-TOF MS: m/z = 432.60 ([M + H] +), Calcd. For $C_{32}H_{20}N_2$: 432.16. 1H NMR(500 MHz, 25 °C, CDCl3, TMS, ppm): δ 8.04(s, 2H), 7.66(d, 2H), 7.56(m, 6H), 7.44-7.33(m, 28H), 7.19(s, 2H); FT-IR(KBr pellet, cm^{-1}): 3049, 2956, 2240, 1591, 1504, 1465, 1419, 1376, 1339, 1299, 1273, 1205, 1189, 1125, 937, 891, 857, 815, 777, 737, 661.

S2. The structure and refinement data of crystal G *of crystal G*

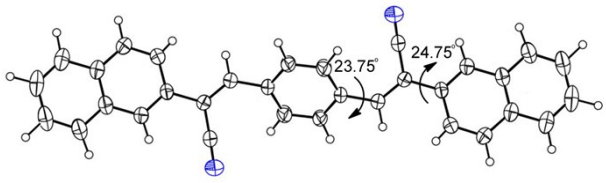

Figure 2. The molecular conformation of PBNA in single crystal G

The crystal G is of the typical monoclinic system, which belongs to the C2/c space group. The density of the crystal is 1.267 mg/m^3. As shown in the Figure 2, the molecule exhibits the trans-configuration with a torsional main carbon chain. The dihedral angle between central benzene ring and the double bond plane is 23.75º, and the one between naphthalene ring and the plane of

double bond is 24.75º.

Table 1. Refinement data of crystal G

Identification code	G		
Empirical formula	$C_{32}H_{20}N_2$	**γ/°**	90
Formula weight	432	**Z**	4
T/K	298	**Density/Mg/m3**	1.267
Crystal system	monoclinic	**M(Mo Kα)/mm-**	0.074
space group	C2/c	**Reflections**	10567
a/Å	46.530	**Independent**	2589
b/Å	6.7629	**R1[I>2σ(I)]**	0.0486
c/Å	7.2639	**wR2[I>2σ(I)]**	0.1476
α/°	90.00	**R1(all data)**	0.0867
β/°	97.22	**wR2(all data)**	0.1580