

Electronic Supplementary Information

of

Formation and properties of liquid crystalline supramolecules with anisotropic fluorescence emission

Jun Wu^a, Zeyuan Yi^a, Xuemin Lu^{a*}, Shuangshuang Chen^a and Qinghua Lu^{a,b*}

^a School of Chemistry and Chemical Engineering, ^bState Key Laboratory of Metal Matrix Composites, Shanghai Jiao Tong University, Shanghai, 200240, P. R.China.

Corresponding Author: E-mail: qhl@sjtu.edu.cn; xuemilu@sjtu.edu.cn.

Table of Contents

Experimental Section

Scheme S1 The synthetic route of TPE6N and the structure of CP91-TPE6N.

Fig. S1 The IR spectra of TPE6N and CP91-TPE6N.

Fig. S2 ¹H NMR spectra of TPE6N and CP91-TPE6N.

Fig. S3 The heating (black) and cooling (red) DSC curves of CP91-TPE6N.

Fig. S4 POM images of CP91-TPE6N at (a) 75 °C under the s heating process and (b) 55 °C under the cooling process.

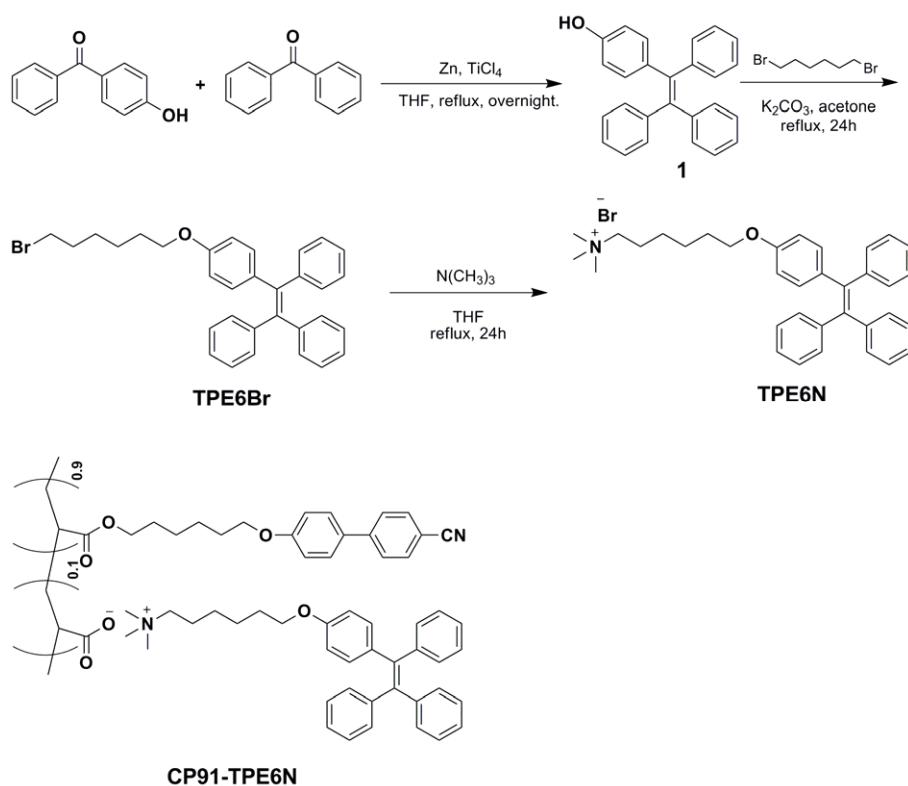
Fig. S5 Polarized UV-vis spectra of CP91-TPE6N oriented film before and after annealing at 65 °C for 15 min. // and ⊥ represents the direction parallel and perpendicular to the rubbing direction.

Fig. S6 Polarized FTIR spectra of CP91-Stil (a) and CP91-TPE (b) in the range of 1350-1850 cm⁻¹.

Reference

Experimental Section

The synthesis of TPE6N and CP91-TPE6N was according to the scheme S1. The synthesis of 1-(4-hydroxyphenyl)-1,2,2-triphenylethene (**1**) was previously reported.¹ The preparation of CP91-TPE6N was according to the procedure of CP91-TPE.



Scheme S1 The synthetic route of TPE6N and the structure of CP91-TPE6N.

Synthesis of 1-(4-(6-bromohexyloxy)phenyl)-1,2,2-triphenylethene (TPE6Br)

A mixture of **1** (3 mmol), 1,6-dibromohexane (5 mmol), potassium carbonate (5 mmol), and acetone was refluxed with stirring for 24 h. The residue was filtered off and washed with ethyl acetate. The organic solvent was removed from the combined filtrate and washings under reduced pressure. The residue purified by flash silica gel column to remove the unreacted 1,6-dibromohexane. Then the crude product was directly used in the next step.

Synthesis of N,N,N-trimethyl-6-(4-(1,2,2-triphenylvinyl)phenoxy)hexan-1-aminium bromide (TPE6N)

The crude TPE6Br was dissolved in 30 mL tetrahydrofuran. Then 33% trimethylamine alcoholic solution (10 mmol) was added to the solution. The mixture was heated to reflux for 24 h. Most of the solvent was removed under reduced pressure. The resulting thick solution was precipitated in ethyl acetate. The product was obtained by filtration and washed with ethyl acetate for 3 times. The filter cake was dried under vacuum to give TPE6N in total yield: 55%. ^1H NMR (DMSO- d_6 , δ (ppm)): 7.06-7.15 (m, 9H, 9 \times ArH), 6.91-6.97 (m, 6H, 6 \times ArH), 6.83 (d, 2H, 2 \times ArH), 6.66 (d, 2H, 2 \times ArH), 3.84-3.87(t, 2H, Ar-CH₂), 3.25-2.29 (m, 2H, N-CH₂), 3.03 (s, 9H, N(CH₃)₃), 1.64-1.70 (m, 4H, 2 \times CH), 1.38-1.46 (m, 2H, CH₂), 1.27-1.33 (m, 2H, CH₂).

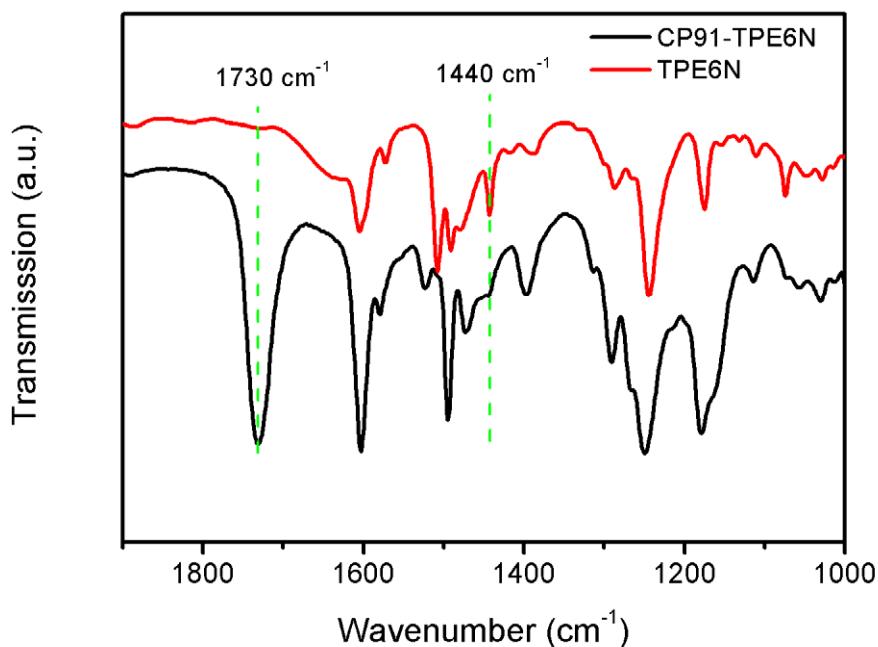


Fig. S1 The IR spectra of TPE6N and CP91-TPE6N.

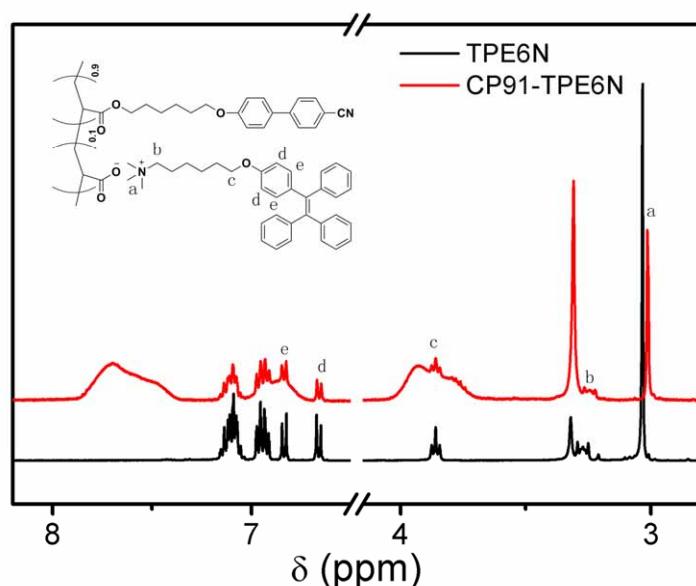


Fig. S2 ^1H NMR spectra of TPE6N and CP91-TPE6N.

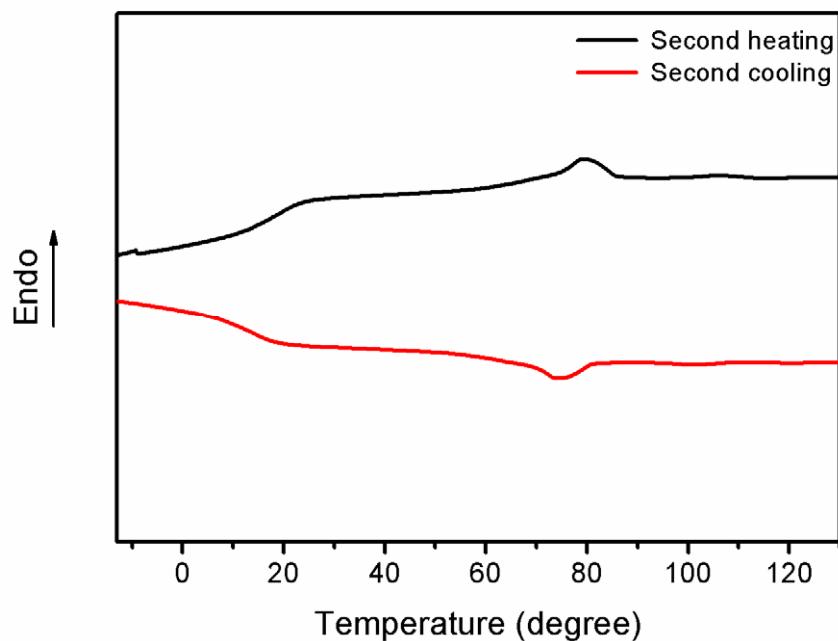


Fig. S3 The heating (black) and cooling (red) DSC curves of CP91-TPE6N.

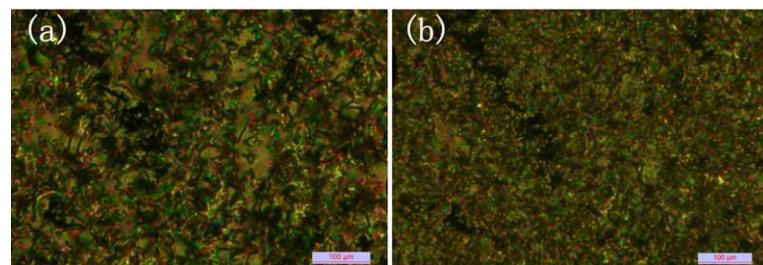


Fig. S4 POM images of CP91-TPE6N at (a) 75 °C under the heating process and (b) 55 °C under the cooling process.

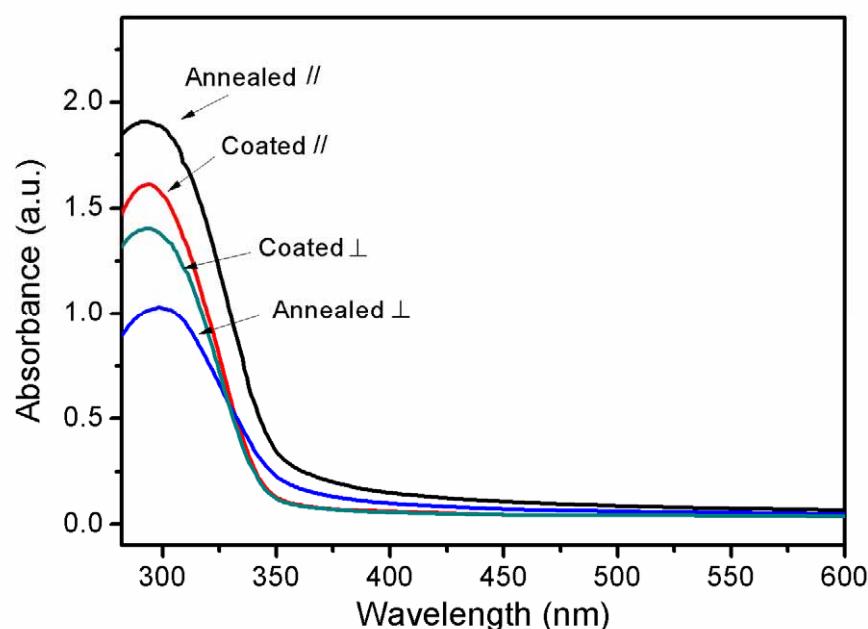


Fig. S5 Polarized UV-vis spectra of CP91-TPE6N oriented film before and after annealing at 65 °C for 15 min. // and ⊥ represents the direction parallel and perpendicular to the rubbing direction.

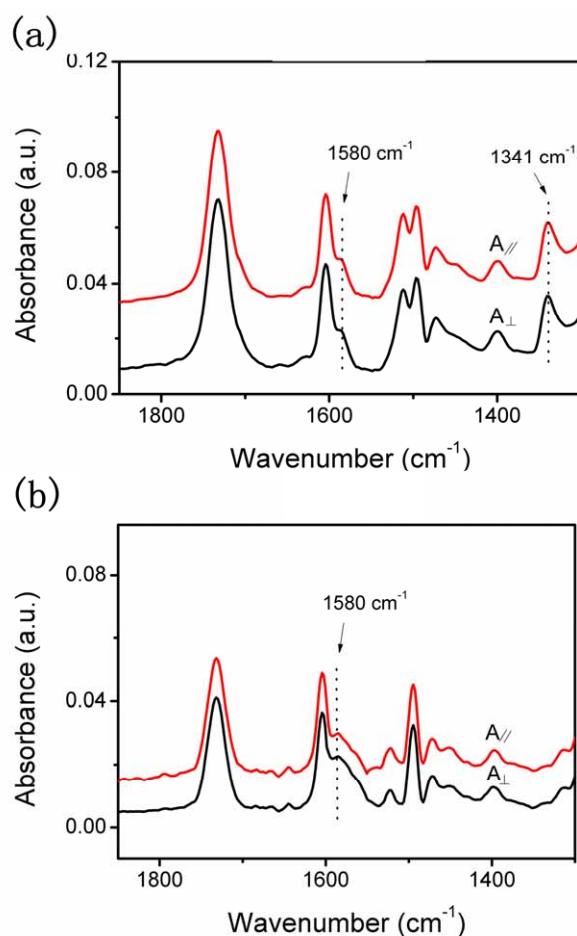


Fig. S6 Polarized FTIR spectra of CP91-Stil (a) and CP91-TPE (b) in the range of 1350-1850 cm^{-1} .

Reference

1. Q. Zhao, K. Li, S. Chen, A. Qin, D. Ding, S. Zhang, Y. Liu, B. Liu, J. Z. Sun and B. Z. Tang, *J. Mater. Chem.*, 2012, **22**, 15128-15135.