Supplementary material (ESI) for Journal of Materials Chemistry

Supporting information (SI)

Novel host material for single-component white organic light-emitting diodes based on 9-naphthylanthracene derivatives

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The definition of some related terms in the paper:

Electromer is an excited state complex of a pair of molecules under electric excitation, in which one carried an excess electron while the other carried a hole; Exciplex is a metastable complex formed by associative excited state interactions between two different molecules; Excimer is a metastable complex formed by associative excited state interactions between two same molecules; Aggregate is the component of composite materials used to resist compressive stress, in which the monomer is the ground state.

Experimental section:

9-(1-Naphthyl)anthracene (1a). Yield 90%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.59 (s, 1H), 8.09 (d, J = 8.8Hz, 2H), 7.99-8.06 (m, 2H), 7.68-7.70 (m, 1H), 7.38-7.53 (m, 6H), 7.18-7.26 (m, 3H), 7.05-7.07 (d, 1H); FAB-MS: calcd MW: 304.4 ; m/z = 304[M^+ for $C_{24}H_{16}$]. The compound was synthesized according to the literature procedure.[1]

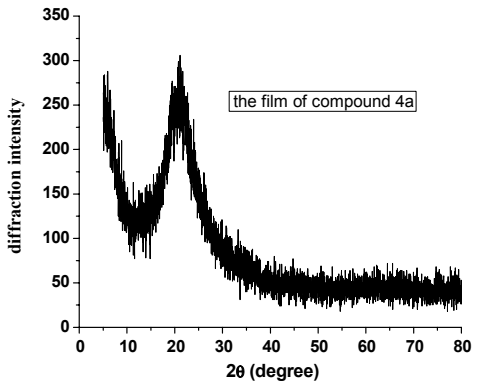
9-(2-Naphthyl)anthracene (1b). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.52 (s, 1H), 7.99-8.09 (m, 4H), 7.88-7.93 (m, 2H), 7.66-7.69 (m, 2H), 7.54-7.61 (m, 3H), 7.44-7.49 (m, 2H), 7.29-7.34 (m, 2H); FAB-MS: calcd MW: 304.4 ; m/z = 304 [M^+ for $C_{24}H_{16}$]. The compound was synthesized according to the literature procedure.[1]

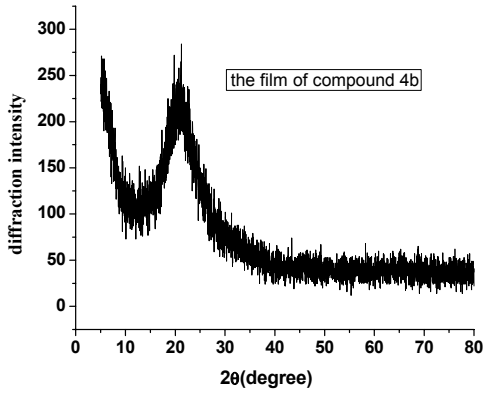
9-(1-Naphthyl)-10-(bromo)anthracene (2a). yield 91%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.63-8.66 (d, 2H), 7.98-8.07 (m, 2H), 7.38-7.70 (m, 7H), 7.16-7.29 (m, 3H), 7.04 (m, 1H); FAB-MS: calcd MW, 383.3, m/z = 384 [M^+ for $C_{24}H_{15}Br$]. The compound was synthesized according to the literature procedure.[1]

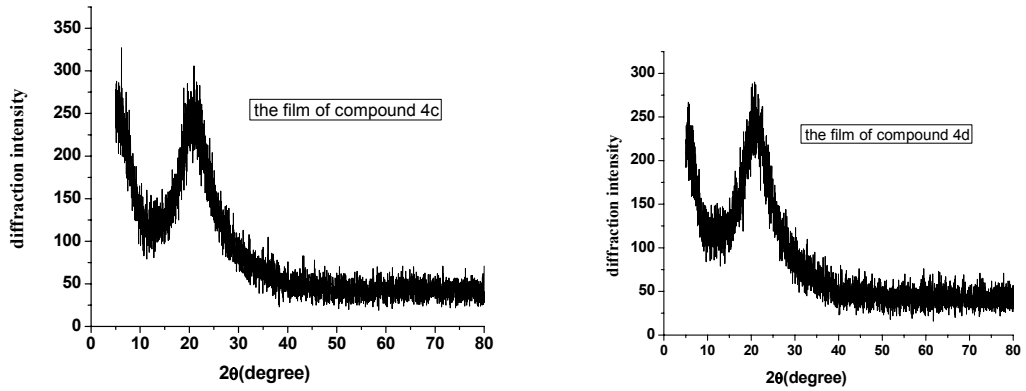
9-(2-Naphthyl)-10-(bromo)anthracene (2b). yield 89%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.61-8.63 (d, J = 8.8Hz, 2H), 7.99-8.075 (m, 2H), 7.84-7.89 (m, 2H), 7.64-7.66 (d, J = 8.8 Hz, 2H), 7.56-7.60 (m, 4H), 7.50-7.52 (m, 1H), 7.32-7.35 (m, 2H); FAB-MS: calcd MW, 383.3, m/z = 384 [M^+ for $C_{24}H_{15}Br$] . The compound was synthesized according to the literature procedure.[1]

The X-ray diffraction of the film of 4a, 4b, 4c and 4d:

All the evaporated film of **4a, 4b, 4c** and **4d** show only a broad halo in their X-ray diffraction patterns (see supporting information) indicates that they form uniform amorphous films by vacuum deposition.







The DSC of coumpound 4a and 4b

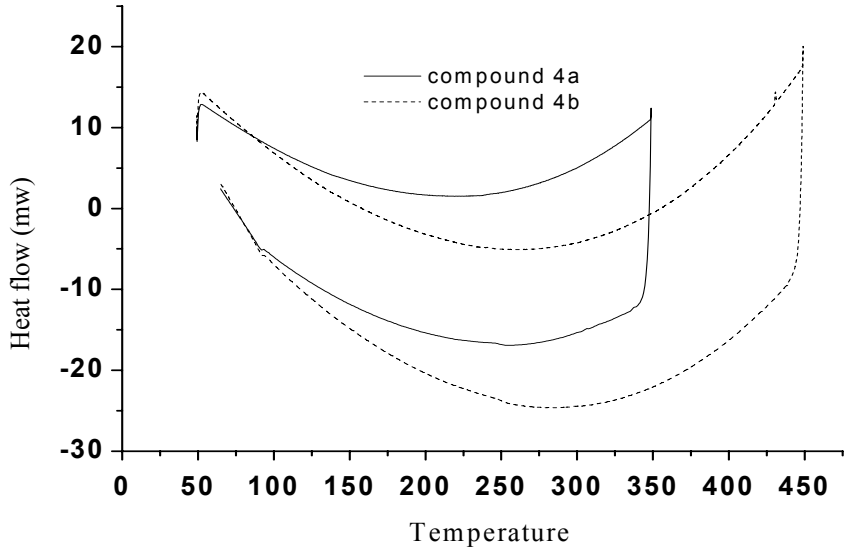


Fig. 1 The DSC spectra (differential scanning calorimetry) of the compound **4a** and **4b**. (20mg sample was added to the pan, then it is heated up to 350 ºC or (450 ºC)at 20 ºC/min and go through a quick cooling at 50 ºC/min by the ice-bath, then scan it and collect the data).

Reference:

[1] S. R.Conley, L. L. Cosimbescu, W. B.Vreeland, *U.S. Pat. Appl. Publ*. **2003**, U.S. 20050245752