An ambipolar host material provides highly efficient saturated-red PhOLEDs possessing simple device structures

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Electronic Supplementary Information



Scheme S-1: The synthesis of red emitter Mpq₂Iracac

Synthesis of the red emitter (Mpq₂Iracac): 3-Methyl-2-phenylquinoline (1) (5.9 g, 26.93 mmol), which was synthesized according to the literature procedures ^[11], and iridium trichloride hydrate (4.46 g, 12.24 mmol) dissolved in a mixture of 2-ethoxylethanol (180 mL) and H₂O (60 mL) were refluxed overnight ^[2]. The solution was cooled to room temperature, and the red precipitate was collected and washed with methanol (30 mL). The vacuum-dried dichloro-bridged iridium dimmer complex (**2**) was used for the next step without further purification. A mixture of 2,4-pentandione (1.01 g, 10.08 mmol), Na₂CO₃ (2.14 g, 20.19 mmol) and iridium dimmer (**2**) (5.35 g 4.03 mmol) in 2-ethoxylethanol (280 mL) was heated to 100 °C for 24 h. After cooling to room temp., the mixture was extracted twice with CH₂Cl₂. The combined organic solution was washed with brine and dried over MgSO₄, the product was isolated as red solid by recrystallisation from DMSO (60 mL) to afford Mpq₂Iracac (**3**), (2.26 g, 77%). M.p. = 329-330 °C; ¹H NMR (Aceton-d⁶, 400 MHz) δ 7.49 (s, 2H), 7.3 (t, *J* = 8.2 Hz, 4H), 7.05 (d, *J* = 8 Hz, 2H), 6.66 (t, *J* = 8 Hz, 2H), 6.59 (t, *J* = 8 Hz, 2H), 6.08 (t, *J* = 8 Hz, 2H), 5.72 (t, *J* = 8 Hz, 2H), 5.60 (d, *J* = 7.6 Hz, 2H), 3.59 (s,

1H), 2.22 (s, 6H), 1.73(s, 1H), 0.50(s, 6H); ¹³C NMR (CD₂Cl₂, 100 MHz) δ 185.5, 170.4, 152.4, 149.1, 148.1, 140.8, 137.1, 129.8, 129.6, 129.2, 128.1, 127.1, 126.9, 126.5, 120.9, 99.5, 41.7, 28.3, 24.1; HRMS (m/z, ESI⁺) Cacld for C₃₇H₃₁¹⁹³IrN₂O₂ 728.2015, found 728.2015

Reference:

[1] Taguchi, K. Sakaguchi, S. and Ishii, Y., Tetrahedron Lett. 2005, 46, 4539.

[2] Nonoyama, M. Bull. Chem. Soc. Jpn. 1974, 47, 767.



Fig. S-1. Cyclic voltammagram of **D2ACN**. The oxidation potentials were determined in CH_2Cl_2 solution (1.0 mM) containing 0.1 M tetra-*n*-butylammonium hexafluorophosphate (TBAPF₆) as a supporting electrolyte. The reduction potentials were determined in THF solution (1.0 mM) containing 0.1 M tetra-*n*-butylammonium perchlorate (TBAP). A glassy carbon electrode and a platinum wire were used as the working and counter electrodes, respectively. The ferrocenium/ferrocene redox couples for oxidation (in THF/TBAP) and reduction (in CH₂Cl₂/TBAPF₆) occur at values of $E^{o'}$ of +0.61 and +0.45 V vs. Ag/AgCl (saturated).

In this communication, we present a systematic study of Time-of-Flight Mobility Measurements. carrier-transport properties in vapor-deposited glasses of oligothiophenes by the time-of-flight (TOF) transient photocurrent technique [1]. The samples for the TOF measurement were prepared by vacuum deposition using the structure: glass/Ag(30nm)/ D2ACN (1.5 µm)/ Al(150nm), and then placed inside a cryostat and kept under vacuum. All organic materials were purified by train sublimation before used. The thickness of organic films were monitored in situ with a quarz crystal sensor and calibrated by a profilometer (Tencor Alpha-step 500). A pulsed nitrogen tunable dye laser was used as the excitation light source (to match the absorption of organic films) through the semitransparent electrode (Ag) induced photogeneration of a thin sheet of excess carriers. Under an applied dc bias, the transient photocurrent was swept across the bulk of the organic film toward the collection electrod (Al), and then recorded with a digital storage oscilloscope. Depending on the polarity of the applied bias, selected carriers (holes or electrons) are swept across the sample with a transit time of t_T . With the applied bias V and the sample thickness D, the applied electric field E is V/D, and the carrier mobility is then given by $\mu = D/(t_T E) = D^2/L$ (Vt_{τ}) . Figures S-2(a) and S-2(b) display representative TOF transients for holes and electrons, respectively, measured at room temperature under an applied field of 4.7×10^5 V cm⁻¹. Both transients exhibit dispersive behavior, such that the carrier transit time $(t_{\rm T})$ can be evaluated from the point of intersection of the two asymptotes in the double logarithmic representation [see the insets to Figures S-2(a) and S-2(b)].

¹ P. M. Borsenberger and D. S. Weiss, *Organic Photoreceptors for Imaging Systems*, Marcel Dekker, New York, 1993.



Fig. S-2. Representative TOF transients for D2ACN (1.5 µm): (a) holes; (b) electrons.



Fig. S-3. Power efficiencies of devices incorporating various dopant concentrations, plotted as functions of the current density.