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A new imidazolylquinoline for organic thin film transistor

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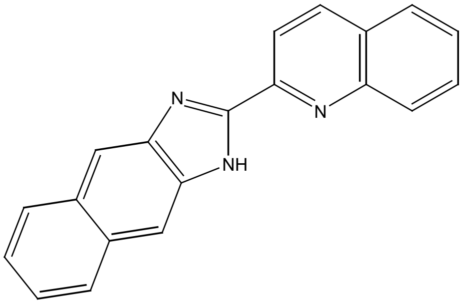
Abstract—A new active electronic material, 2-(naphtho[3,4]imidazol-2-yl)quinoline (NIQ), **1**, has been synthesized and fully characterized. This compound exhibits field-effect carrier mobility and behaves as a p-type semiconductor ($\mu_{FET} = 0.148\ cm^2/V\ s$ at $V_{DS} = 10$ V). NIQ and its related imidazolylquinoline compounds may have possible applications as active materials in organic thin film transistors.

Organic electronic devices (OED's) have made extreme progress over the last few years and investigations into synthesizing new active organic materials for applications in organic thin film transistors (TETs) have attracted great attention recently.[1] In this letter, preliminary results of synthesis, structure, and field-effect properties for a new imidazolylquinoline compound are reported.



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The white compound 2-(naphtho[3,4]imidazol-2-yl)-quinoline (NIQ), **1**, was isolated in ca. 80% yield from the reaction of quinoline-2-carboxylic acid with 2,3-diaminonaphthalene and polyphosphoric acid (PPA).[2] Its structure has been determined by ^{1}H NMR, elemental analysis, and X-ray crystallography.[3] Figure 1 shows the ORTEP diagram of **1**. The dihedral angle between imidazol ring and quinoline ring is 5°, indicating that this molecule approximates to a planar structure, which is stabilized by an intramolecular N(2)–H···N(3) (H–N = 2.622 Å) hydrogen bond, and the delocalization of π-electrons of the heterocyclic system. Figure 2 shows a packing diagram for **1**. The interplanar distances between imidazol ring and quinoline moiety are in the range 3.4–3.5 Å, which imply that the intermolecular charge transfer interaction (ICT)[4] may play an important role in producing face-to-face π–π stacking interactions. The fact that the UV–vis spectrum of NIQ thin film obtained by vacuum deposition onto quartz substrates is different from that measured in solution shows the existence of ICT in solid state.[5] As shown in Figure

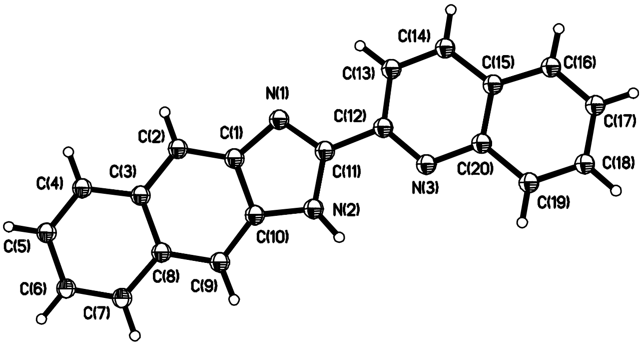

Figure 1. ORTEP plot for compound **1**.

Keywords: Imidazolylquinoline; Organic TFT; Field effect.

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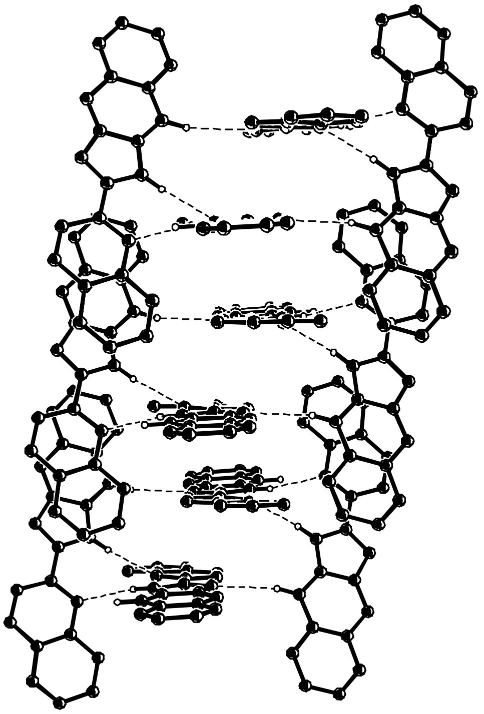

Figure 2. A view of the packing diagram of **1**.

2, the molecules are self-organized by extensive intermolecular N(2)–H···N(3) (H–N = 2.307 Å) hydrogen bonds between the naphtho[3,4]imidazol N–H groups and quinoline nitrogen atoms, leading to the formation of an infinite three-dimensional supramolecular architecture, which provides a carrier channel that can be varied by the electric field.[6] The TGA scans under nitrogen for NIQ powder show that NIQ exhibits an onset for degradation at 350 °C, and no weight loss was observed at lower temperature. The weight loss of 5% occurs at 403 °C, indicating that NIQ is quite stable under nitrogen.

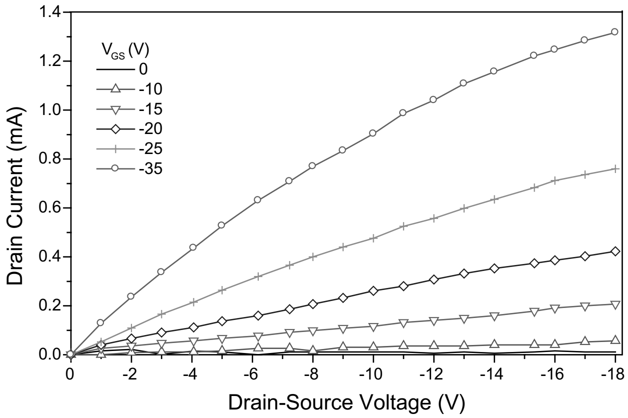

Figure 3. FET characteristics of NIQ TFT in the accumulation regime.

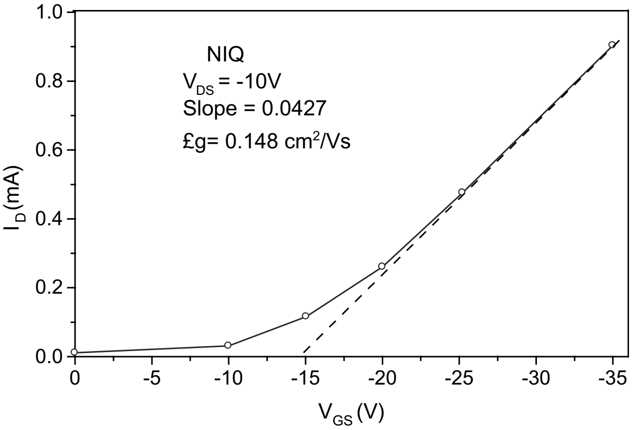

Figure 4. Plot of drain current versus gate voltage at a constant drain voltage of 10 V from the NIQ TFT.

The NIQ-based TFT device was fabricated using heavily doped silicon wafer as the substrate and gate electrode, with thermally grown silicon oxide (thickness 600 nm) as the TFT gate dielectric. Gold source and drain contacts (thickness 100 nm) were deposited onto the SiO_2 surface by thermal evaporation through a shadow mask, which defined a channel length (*L*) and width (*W*) of 40 μm and 2 cm, respectively. Finally, a 200 nm title compound purified by vacuum gradient sublimation[7] was deposited over the source and drain contacts through a mask by thermal evaporation under 5×10^{-5} Pa. Transistor *IV* characteristics have been measured by Keithley 2400 source meter at room temperature. Figure 3 shows the current–voltage curves, $I_D = f(V_D)$, of a NIQ-based TFT for various gate voltage (V_G). The negative gate voltages indicate that the device operates in the accumulation regime and the majority carriers of this device are positive holes, showing that NIQ is a p-type semiconductor.[8] Furthermore, the fact that the highest occupied molecular orbital (HOMO) energy level of NIQ, 5.18 eV, measured form the cyclic voltammetry (CV)[9] is close to the valence band of gold (5.1 eV) also implies that NIQ is a p-type material. The mobility, μ, can be calculated using the linear regime from the transconductance, $g_m = (WC_i/L)\mu V_D$, obtained by plotting I_D versus gate voltage at a constant drain voltage and equating the value of the slope[10] where C_i is the capacitance per unit area of the insulating layer (600 nm thermally grown SiO_2 with $C_i = 5.75 \times 10^{-9}$ F cm^{-2}). Figure 4 shows such a plot and the calculated average mobility value is 0.148 cm^2/V s for V_{DS} = 10 V.

In summary, a new organic active compound of imidazolylquinoline, NIQ, has been synthesized and structurally characterized. This new material is a p-type semiconductor and exhibits a mobility of 0.148 cm^2/V s at V_{DS} = 10 V. Because of the performance of high thermal stability and excellent electrical characteristics, NIQ and its related imidazolylquinoline compound may have possible application in the organic thin film transistors.

Acknowledgements

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References and notes

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2. Quinoline-2-carboxylic acid (20.0 mmol, 3.46 g), 2,3-diaminonaphthalene (20.0 mmol, 3.16 g), and polyphosphoric acid (PPA, 20 mL) were added to a flask. The mixture was heated at 200 °C for 4 h. After cooling to room temperature, the residue was slowly added to deionized water (500 mL) with stirring. The solid was collected by suction filtration and purified by column chromatography. Colorless crystals of **1** were obtained in 80% yield. ^{1}H NMR (500 MHz, DMSO-d_6, 293 K), δ ppm: 7.38 (2H, m), 7.67 (1H, m), 7.86 (1H, m), 8.0 (2H, m), 8.04 (1H, d, $J = 8$ Hz), 8.19 (1H, s), 8.21 (1H, d, $J = 8$ Hz), 13.36 (1H, s). ^{13}C NMR (500 MHz, DMSO-d_6, 293 K), δ ppm: 119.34, 123.39, 127.34, 127.56, 127.90, 128.13, 130.18, 137.14, 147.09, 148.19, 154.54. Calcd for $C_{20}H_{13}N_3$ (MW = 295.33): C, 81.36; H, 4.41; N, 14.24. Found: C, 81.20; H, 4.40; N, 14.20. UV (DMF), λ nm: 230, 271, 356. UV (thin film), λ nm: 262, 319, 348, 392, 411.
3. Crystal data for **1**, $C_{20}H_{13}N_3$, $M = 295.33$, orthorhombic, space group *Pcca*, $a = 26.4220(5)$, $b = 8.4550(2)$, $c = 13.0920(3)$ Å, $V = 2924.73(11)$ Å^3, $Z = 8$, $D_c = 1.341$ g cm^{-3}, $\mu = 0.081$ mm^{-1}, $R_1 = 0.0512$, and $wR_2 = 0.1235$ with $I > 2\sigma(I)$. The crystallographic data (excluding structure factors) for the structure in this paper has been deposited with the Cambridge Crystallographic Data Centre as supplementary publication number CCDC 249158. Copies of the data can be obtained, free of charge, on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, NK [fax: +44(0) 1223 336033 or e-mail: deposit@ccdc.cam.ac.uk].
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