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# Novel multiresonant diindolophenazine fluorophore as a hole-transport organic semiconductor

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## S1. Synthetic and characterization details

All solvents and starting materials were purchased from commercial resources and were used as received unless otherwise stated. 3,6-Diphenyl-9*H*-carbazole were synthesized according to previous report.[S1] $^1$H and $^{13}$C Nuclear magnetic resonance (NMR) spectroscopy was recorded on a Bruker AVANCE III 400 WB spectrometer at room temperature. Mass spectra (MALDI-TOF-HRMS) were performed on a Bruker SolariX XR 15T. Elemental analysis (C, H, N) was carried out with an Elementar Vario MICRO cube elemental analyzer.

*1-Bromo-3,6-diphenyl-9*H*-carbazole* **2**. A mixture of 3,6-diphenyl-9*H*-carbazole (9.66 g, 30.2 mmol) and *N*-bromosuccinimide (5.33 g, 29.9 mmol) in DMF (50 ml) was stirred at room temperature for 12 h. The reaction mixture was diluted with dichloromethane, washed with brine and evaporated under reduced pressure. The crude product was purified by column chromatography on silica gel using petroleum ether–dichloromethane (5 : 1) as an eluent ($R_f$ 0.23) to afford **2** (8.23 g, 69%) as a white powder. $^1$H NMR (300 MHz, $CDCl_3$) $\delta$: 8.32 (d, *J* 1.7 Hz, 1H), 8.27 (d, *J* 1.2 Hz, 2H), 7.87 (d, *J* 1.5 Hz, 1H), 7.79–7.68 (m, 5H), 7.59–7.48 (m, 5H), 7.44–7.36 (m, 2H). $^{13}$C NMR (75 MHz, $CDCl_3$) $\delta$: 141.73, 140.83, 139.01, 137.95, 134.69, 133.81, 128.89, 128.84, 127.58, 127.32, 127.02, 126.74, 126.33, 125.10, 124.42, 119.35, 117.96, 111.39, 104.45.

*2,5,10,13-Tetraphenyldiindolo[3,2,1-*de*:3',2',1'-*kl*]phenazine* (**PhDIPz**). A mixture of **2** (4.1 g, 10.4 mmol), CuI (0.4 g, 2.1 mmol), 18-crown-6 (0.42 g, 2.1 mmol) and anhydrous $K_2CO_3$ (2.15 g, 15.6 mmol) in *o*-DCB (20 ml) was heated to 180 °C and stirred for 24 h under the protection of argon. After cooling down to room temperature, the bulk was diluted with ethanol (100 ml). The formed precipitate was filtered off and washed successively with ethanol, 1 N hydrochloric acid, water, and ethanol. The crude product was extracted by Soxhlet extractor with toluene, the obtained solution was concentrated to afford PhDIPz (1.4 g, 42%) as a yellow powder. $^1$H NMR could not be obtained because of its insolubility. MS (MALDI-TOF), *m*/*z*: 634.24273 [M]$^+$ (calc. for $C_{48}H_{30}N_2^+$, *m*/*z*: 634.24035). Found (%): C, 89.98; H, 4.79; N, 4.36. Calc. for $C_{48}H_{30}N_2$ (%): C, 90.82; H, 4.76; N, 4.41.

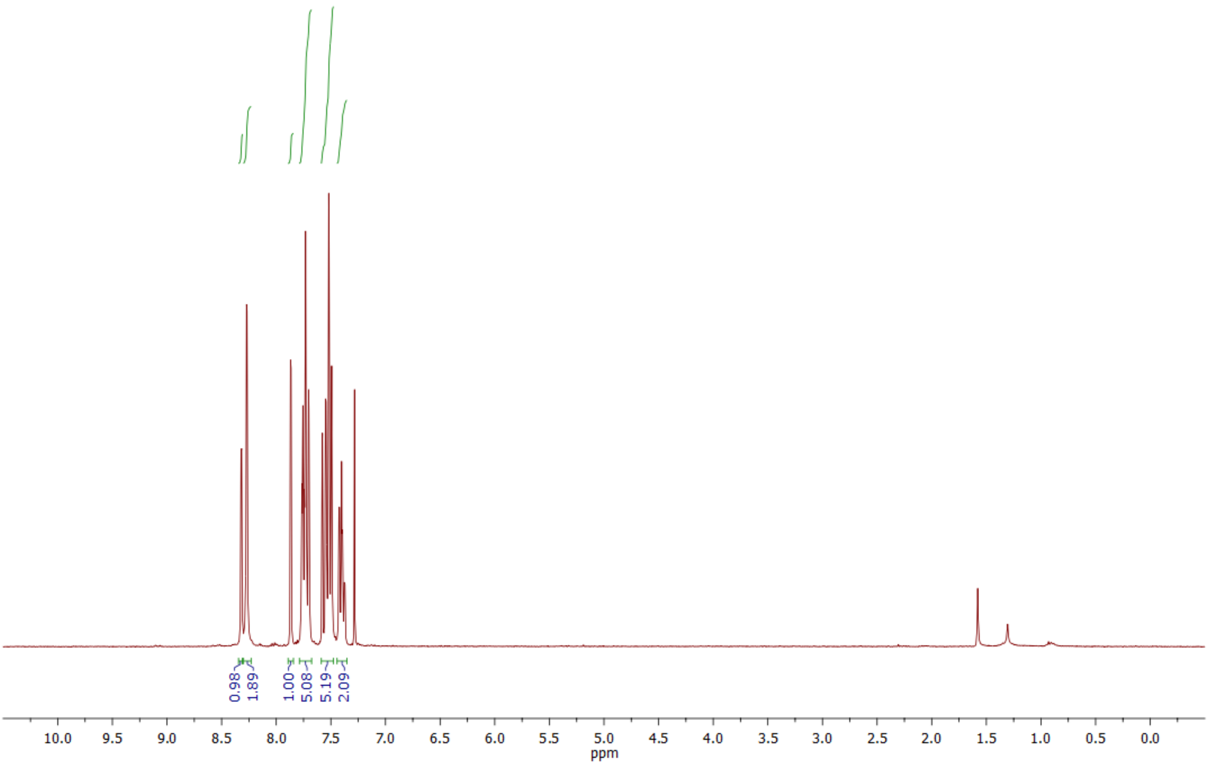

**Figure S1** $^{1}$H NMR spectrum of **2**.

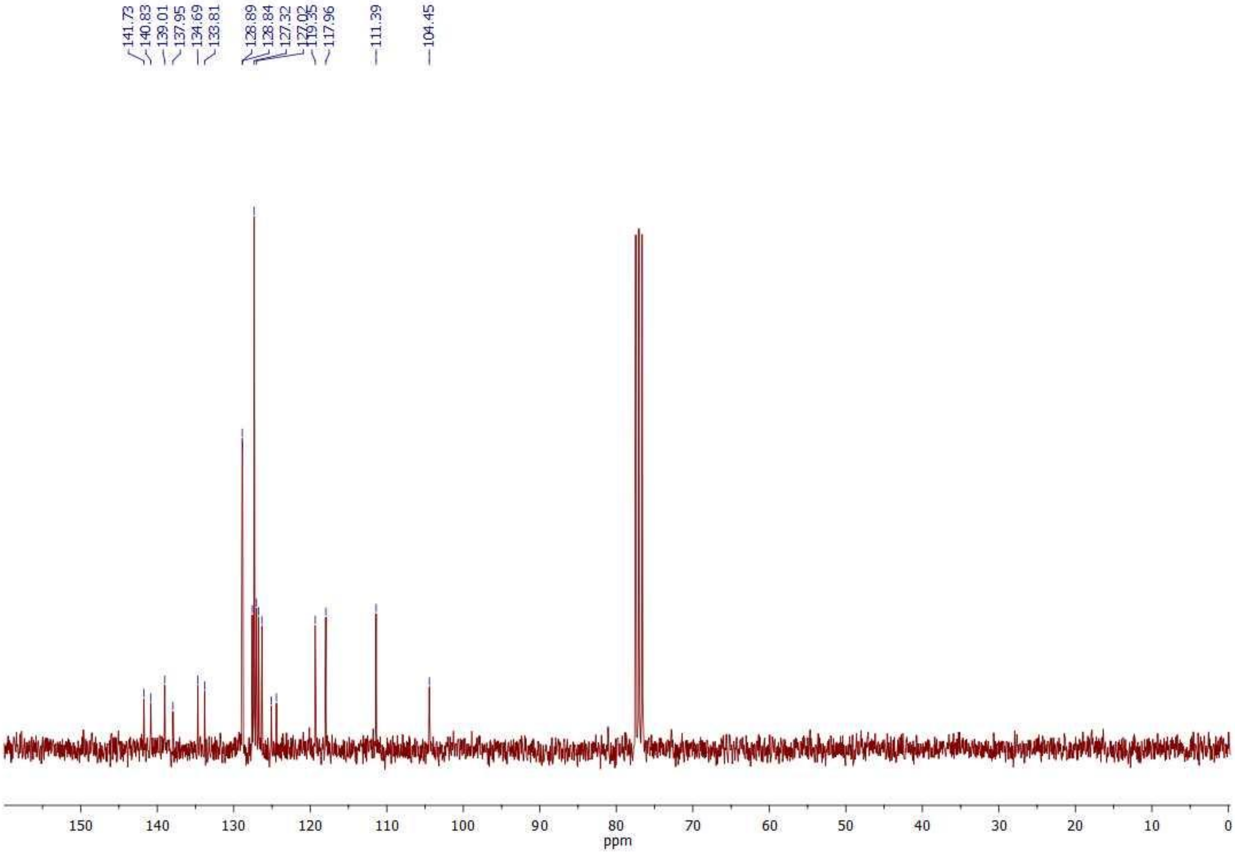

**Figure S2** $^{13}$C NMR spectrum of **2**.

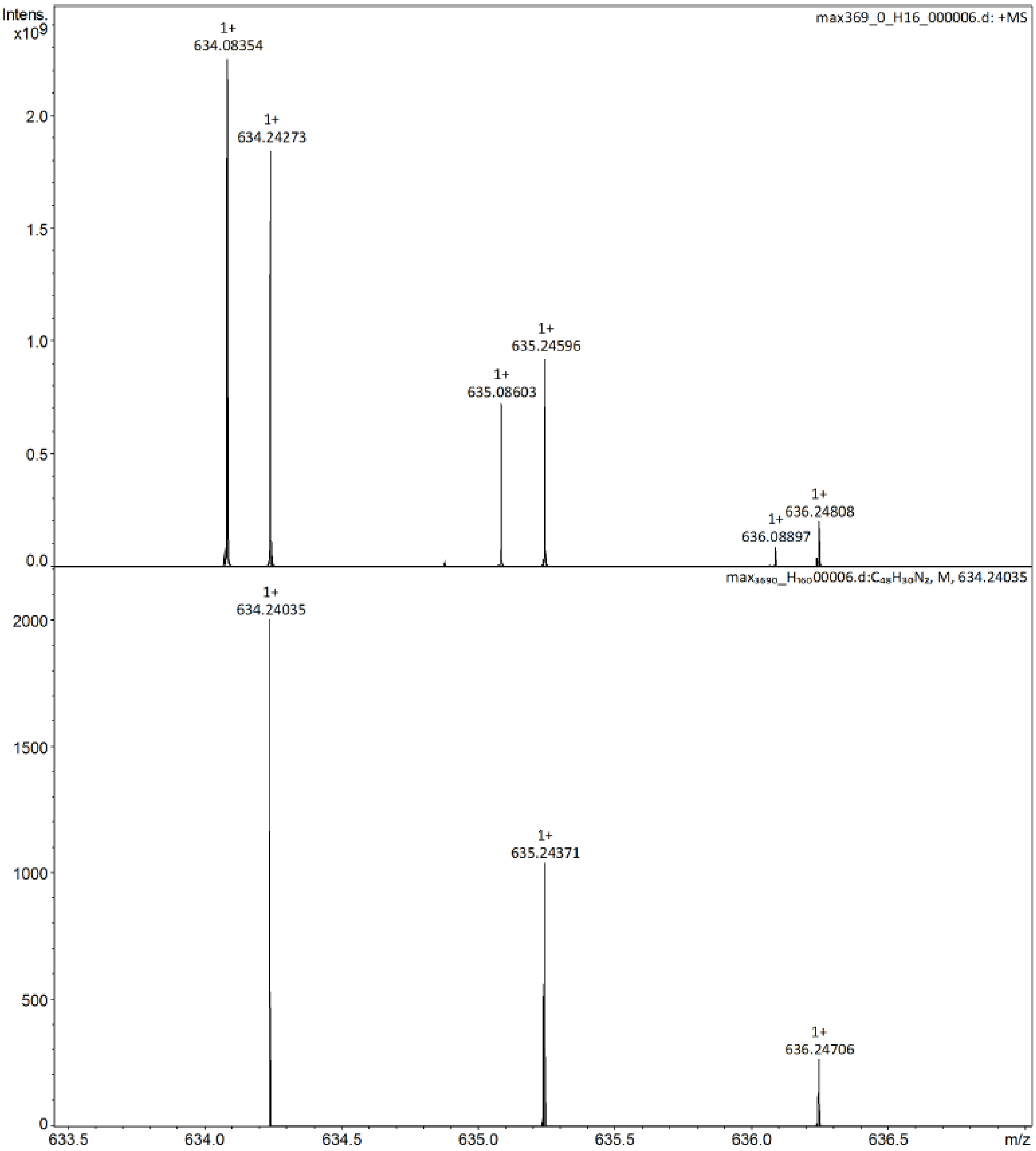

**Figure S3** MALDI-TOF spectrum of **PhDIPz**.

## S2. PL measurements details

PL spectra were recorded using OmniFluo990 fluorescence spectrometer (Zolix Instruments). PL excitation and emission spectra were achieved under excitation of a 75W continuous xenon lamp. PL quantum yield was measured using an integrating sphere. Time-resolved PL measurements were conducted with a picosecond 375 nm diode laser (SSP-MD-PSL-375-40-2, CNI).

## S3. OFETs fabrication and characterization details

Silicon substrates coated with a 300-nm-thick layer of silicon oxide $SiO_2$ and a 50-nm-thick layer of polymethyl methacrylate (PMMA, $M_w \sim 35\,000$) were used. The PMMA layer was deposited on the Si/$SiO_2$ substrates using a TC100 AG spin coater (MTI) at 3000 rpm for 2 min from a 10 g dm$^{-3}$ toluene solution, then the substrates after deposition of PMMA were annealed on a hot plate at 70 °C for 20 h and then at 110 °C for 3 h. An active PhDIPz layer with a thickness of 50 nm was deposited on top of the PMMA layer by thermal vacuum evaporation in a vacuum chamber (Univex 300G, Leybold) at pressure lower than $4 \times 10^{-6}$ mbar with rate about 1 Å $s^{-1}$. The drain and source electrodes, which consisted of a 10-nm-thick $MoO_3$ layer and a 50-nm-thick silver layer, were deposited on top of the active layer through shadow masks. Twenty OFET samples with a channel length of $L = 30$ μm and a channel width of $W = 1$ mm were formed on one substrate.

The measurements of the current–voltage transfer and output characteristics of the fabricated OFET samples were carried out using a source-meter (Keithley SourceMeter 2636A) with a probe station (ProbeStation 100, Printeltech, Moscow, Russia). The charge mobility and threshold voltage were determined from the approximation of the transfer characteristics by the Shockley equations in the linear mode and saturation mode:

$$I_{\mathrm{D}} = \frac{W}{L}\mu_{\mathrm{lin}}C(V_{\mathrm{G}} - V_{\mathrm{T}})V_{\mathrm{D}};\ I_{\mathrm{D}} = \frac{W}{2L}\mu_{\mathrm{sat}}C(V_{\mathrm{G}} - V_{\mathrm{T}})^2,$$

where $\mu_{\mathrm{lin}}$ and $\mu_{\mathrm{sat}}$ are charge mobilities in linear and saturation regime, respectively; $C = 9.9$ nF $cm^{-2}$ is capacitance of the gate dielectric per unit area for a 300-nm-thick $SiO_2$ layer coated with 50-nm-thick PMMA layer both with a permittivity of 3.9; $V_{\mathrm{T}}$ is the threshold voltage. All stages of the fabrication and characterization of the OFET samples were carried out in glove boxes with an inert atmosphere (nitrogen).

## S4. Molecular dynamics simulations details

Molecular dynamics (MD) simulations were carried out using the OPLS-aa force field. Each MD simulation comprised a cubic, amorphous, periodic cell of 7 × 7 × 7 nm, containing 100 PhDIPz molecules. The cells were initially relaxed at 900 K for structural stabilization, followed by NPT relaxation at 600 K with a Berendsen barostat to achieve realistic density. Finally, further NPT relaxation at 298 K established room-temperature configurations. All MD simulations were performed using the Gromacs software package.

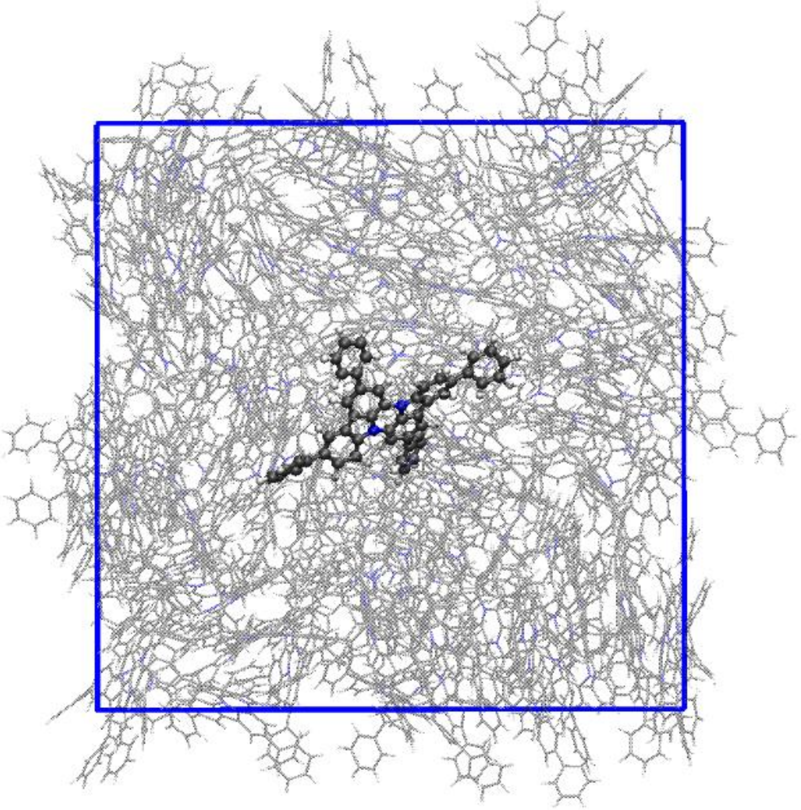

**Figure S4** Molecular dynamic cell of PhDIPz film.

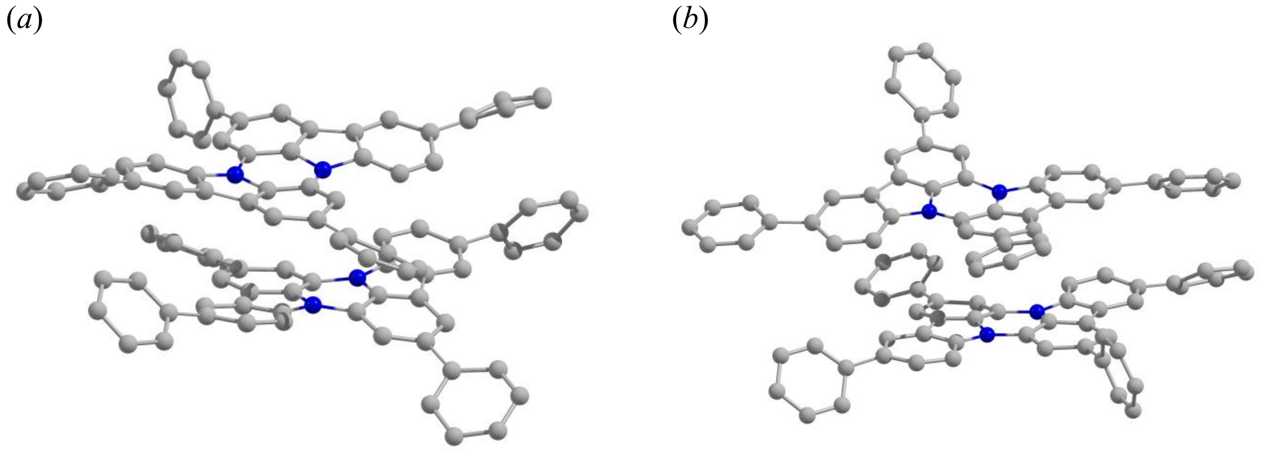

**Figure S5** Relative positions of molecules in dimers exhibiting considerable transfer integrals of (*a*) 66 and (*b*) 68 meV.

## References

S1 B. Liu, Z. Chen, L. Lin, Y. Han, J. Pang and Z. Jiang, *High Perform. Polym.*, 2016, **29**, 575; https://doi.org/10.1177/0954008316655592.