

Peripheral Modification of 1,3,5-Triazine Based Electron-Transporting Host Materials for Blue, Green, Yellow, Red, and White Electrophosphorescent Devices

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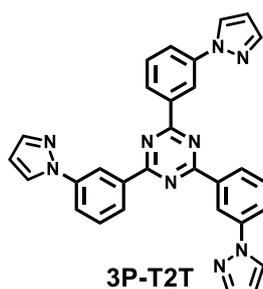
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Supporting Information

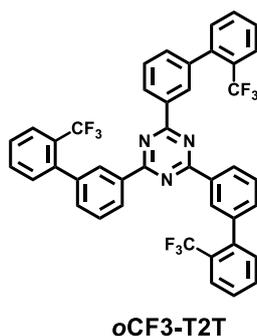
General Experiments

¹H and ¹³C NMR spectra of compounds were collected on a 400 MHz spectrometer at room temperature. Photophysical characteristics of compounds in solutions were collected at room temperature by using 10⁻⁵ M dichloromethane (CH₂Cl₂) solutions of all compounds, which were carefully purged with nitrogen prior to measurements. The thickness of spin-coated films was measured by profilometry. UV-visible absorption spectra were recorded on a spectrophotometer (HITACHI U2800A). PL spectra were measured with a fluorescence spectrophotometer (HITACHI F9500). Reduction potentials of all compounds were determined by cyclic voltammetry (CV) at a scan rate of 100 mV/s in THF solutions (1.0 mM). A glassy carbon electrode and a platinum wire were used as the working electrode and the counter electrode, respectively. All potentials were recorded versus the Ag/AgCl (sat'd) reference electrode and calibrated with the ferrocene/ferrocenium redox couple. Reduction CV was performed using 0.1 M tetra-*n*-butylammonium perchlorate (TBAClO₄) in THF as the supporting electrolyte.

Synthesis



2,4,6-tris(*m*-(1-pyrazolyl)phenyl)-1,3,5-triazine (3P-T2T): A mixture of 2,4,6-tris(3-bromophenyl)-1,3,5-triazine (1.69 g, 3.09 mmol), 1*H*-pyrazole (1.26g, 18.51 mmol), copper(II) oxide (74 mg, 0.93 mmol), tris(acetylacetonato)iron(III) (984 mg, 2.79 mmol), cesium carbonate (6.19 g, 19 mmol), and anhydrous DMF (60 mL) was refluxed under Ar for 72 h. DMF was evaporated and the crude product was dissolved in CHCl₃ and filtered to remove insoluble solids. The organic solution was extracted with brine and dried over MgSO₄. The product was purified by column chromatography on Al₂O₃ (CH₂Cl₂ / Hex / MeOH = 5 / 2 / 0.1) to afford pure 3P-T2T (1.27 g, 81% yield) as a white solid. ¹H NMR (CDCl₃, 400 MHz) δ 9.04 (d, *J* = 1.6 Hz, 3H), 8.72 (dd, *J* = 8.0, 1.6 Hz, 3H), 8.13 (d, *J* = 2.8 Hz, 3H), 8.02 (dd, *J* = 8.0, 1.6 Hz, 3H), 7.82 (d, *J* = 1.6, 3H), 7.69 (t, *J* = 8.0 Hz, 3H), 6.57 (split unsymmetrical triplet, 3H); ¹³C NMR (CDCl₃, 100 MHz) δ 170.5, 140.9, 140.2, 136.8, 129.5, 126.7, 123.2, 119.0, 109.2, 107.7; HRMS (*m/z*, ESI⁺) Calcd for C₃₀H₂₁N₉ 507.1920, found (*M* + H⁺): 508.1996; Anal. Calcd. For C₃₀H₂₁N₉: C, 70.99; H, 4.17; N, 24.84. Found: C, 70.68; H, 4.08; N, 25.03; 3P-T2T was soluble in CH₂Cl₂ and CHCl₃.



2,4,6-tris(*m*-(2-trifluoromethyl)phenyl)-1,3,5-triazine (oCF3-T2T): The mixture of 2,4,6-tris(3-bromophenyl)-1,3,5-triazine (3.47 g, 6.35 mmol), 2-trifluoromethylphenylboronic acid (4g, 21.06 mmol), tetrakis(triphenylphosphine) palladium(0) (1.1 g, 0.95 mmol), tri-*tert*-butylphosphine (33 mL, 0.05 M in toluene), and sodium carbonate (13.5 g, 127 mmol) (60 mL) were dissolved in toluene (75 mL) and deionized water (40 mL) and refluxed under Ar for 48 h. After the removal of toluene, the product was extracted with ethyl acetate and CH₂Cl₂, dried over MgSO₄.

The product was purified by column chromatography on silica (CH_2Cl_2 / Hex = 1 / 2) to afford pure *o*CF₃-T2T (2.92 g, 62% yield) as a white solid. ¹H NMR (CDCl_3 , 400 MHz) δ 8.78 (dt, J = 7.6, 1.6 Hz, 3H), 8.73 (s, 3H), 7.79 (d, J = 7.6 Hz, 3H), 7.62-7.49 (m, 12H), 7.43 (d, J = 7.6 Hz, 3H); ¹³C NMR (CDCl_3 , 100 MHz) δ 171.5, 140.8, 140.3, 135.9, 133.0, 132.1, 131.4, 129.4, 128.4, 128.4, 128.1, 127.6, 126.2, 126.1; HRMS (m/z , ESI^+) Calcd for $\text{C}_{42}\text{H}_{24}\text{F}_9\text{N}_3$ 741.1827, found: 741.1825; Anal. Calcd. For $\text{C}_{42}\text{H}_{24}\text{F}_9\text{N}_3$: C, 68.02; H, 3.26; N, 5.67. Found: C, 67.91; H, 3.13; N, 5.66; *o*CF₃-T2T is soluble in CH_2Cl_2 and CHCl_3 .

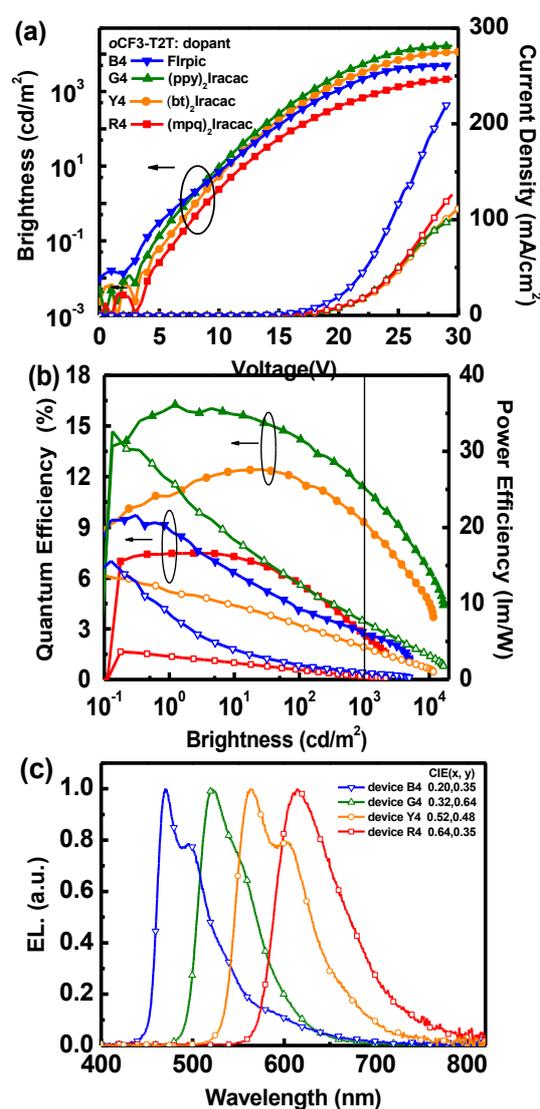
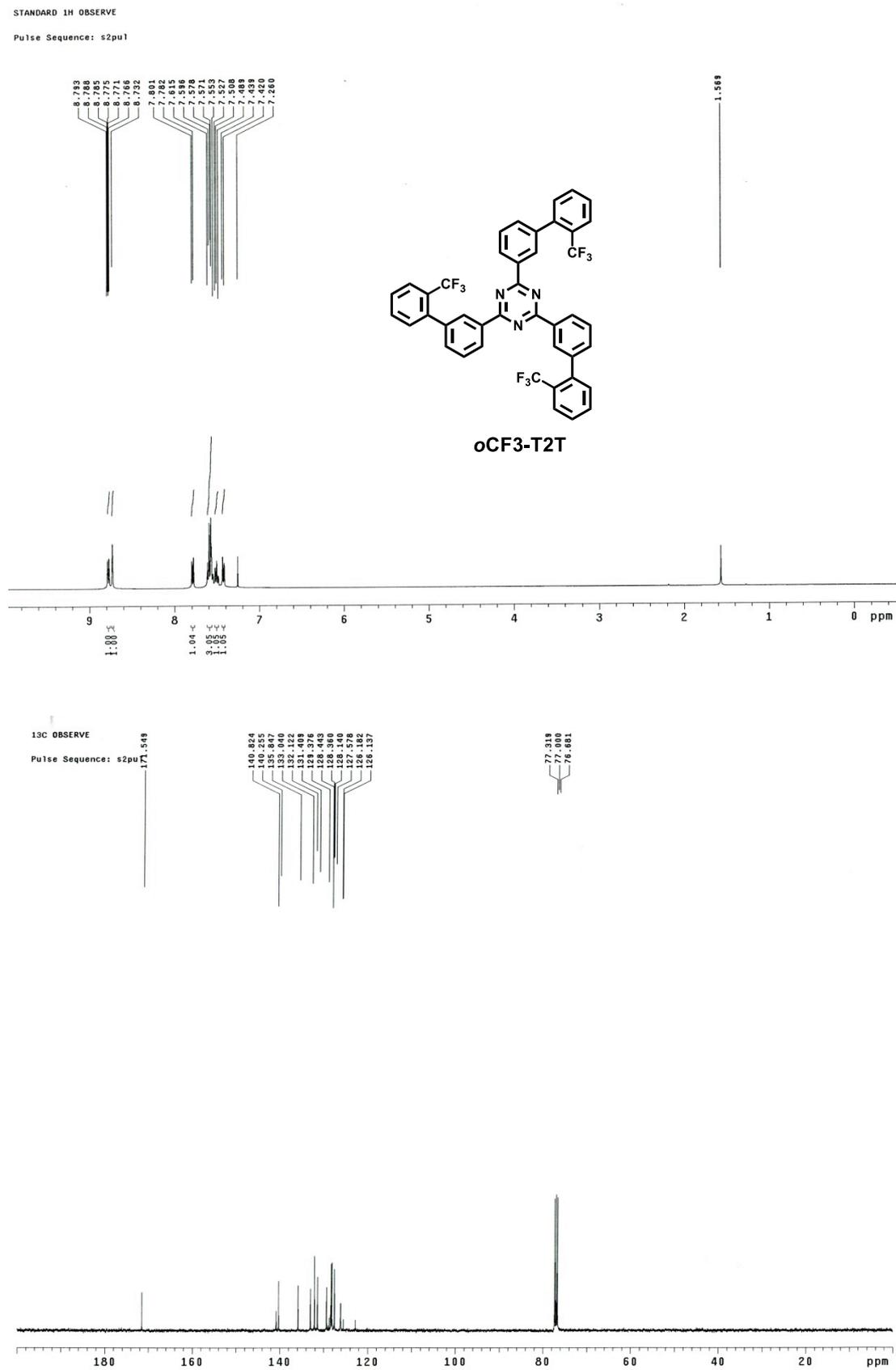


Fig. S1 (a) Current density-voltage-luminance ($J - V - L$) characteristics, (b) external quantum (η_{ext}) and power efficiencies (η_p) as a function of brightness, and (c) EL spectra for devices incorporating *o*CF₃-T2T as host.



^1H (top) and ^{13}C (bottom) NMR spectra of **oCF3-T2T**.