Electronic Supplementary Information

Organic solar cells based on bowl-shape small-molecules

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Homepage: [http://www.ucm.es/info/fullerene/](http://www.ucm.es/info/fullerene/)

Experimental Section

Instrumentation

Solvents were purchased from Sigma-Aldrich and were used without further purification. TruxTTF and truxTTF-CO were prepared according to previously reported synthetic procedures (ref 37 and 38). Absorption studies were performed using a Cary 5000 UV-Vis-NIR spectrometer from Varian. The thickness of blends were measured by employing a KLA-Tencor Alpha-Step D-120 stylus profilometer. Atomic Force Microscopy was performed on a SPM Nanoscope Illa multimode microscope working in tapping mode under ambient conditions.
Solar cell fabrication

PC<sub>61</sub>BM and PC<sub>71</sub>BM were purchased from American Dye Source and used as received. The ITO-coated glasses (Delta technologies, 5-15 Ω) were pre-cleaned stepwise by ultracentrifugation 15 minutes in detergent, deionized water, methanol, acetone and iso-propanol and then by a 20 minutes UV-ozone treatment (Jelight Company, USA). A thin layer of PEDOT:PSS (Clevios P VP AI 4083, 5000 rpm, 30 seconds, ≈ 30 nm) was spin-coated onto the ITO glass and baked at 150 °C for 15 minutes in air. Subsequently, the active layer with varying weight ratios (1:6, 1:4 and 1:2 w/w) was spin-coated at 900 rpm from chlorobenzene:o-DCB (1:3 v/v) solutions. TruxTTF or truxTTF-CO:PC<sub>61</sub>BM or PC<sub>71</sub>BM (1:6, 1:4 and 1:2 w/w) was spin-coated at 900 rpm. Then the devices were transferred to a N<sub>2</sub> filled glove box (< 0.1 ppm O<sub>2</sub> and < 0.1 ppm H<sub>2</sub>O) for further processing. The photoactive layer was annealed at 70 °C for 10 minutes followed by thermal evaporation 60 nm of aluminum (1 x 10<sup>-6</sup> mbar) as negative electrode with a shadow mask of 4 mm<sup>2</sup>. The current-voltage characteristics of the devices were measured by using a computer-controlled Keithley 2420 source unit under 1 sun, AM1.5G spectrum from a solar simulator (Photo Emission Tech CT100) by using a Xenon-lamp at 100 mW cm<sup>-2</sup> as light source and calibrated with a Si-reference cell. The incident photon to current efficiency was recorded using a Bentham PVE300 model.
Figure S1. UV/vis spectra as obtained during the titration of (a) truxTTF (1.15 x 10^-4 M) with PC_61BM (4.9 x 10^-4 M) and (b) truxTTF (1.15 x 10^-4 M) with PC_71BM (4.37 x 10^-4 M), in chlorobenzene at room temperature. Each addition corresponds to 0.1 equiv.
Figure S2. UV/vis spectra as obtained during the titration of (a) truxTTF-CO ($1.44 \times 10^{-4}$ M) with PC$_{61}$BM ($7.14 \times 10^{-4}$ M). Each addition corresponds to 0.2 equiv. (b) truxTTF ($1.15 \times 10^{-4}$ M) with PC$_{71}$BM ($7.48 \times 10^{-4}$ M), in chlorobenzene at room temperature. Each addition corresponds to 0.24 equiv.
Figure S3. UV-vis absorption spectra of truxTTF and truxTTF-CO in diluted chloroform solutions.

Figure S4. Current density-voltage (J-V) curves of the blend truxTTF:PC_{71}BM (1:6) w/w with and without DIO.
Figure S5. Current density-voltage ($J$-$V$) curves of the blend truxTTF-CO:PC$_{71}$BM (1:4) w/w with and without DIO.
Figure S6. Tapping mode AFM height and their profile roughness (1 μm x 1μm) of blends films spin-coated from chlorobenzene:o-DCB of (a and b) truxTTF:PC₆₁BM (1:6), (c and d) truxTTF:PC₇₁BM (1:6), (e and f) truxTTF-CO:PC₆₁BM (1:4) and (g and h) truxTTF-CO:PC₇₁BM (1:4).