Supporting information

A triazatruexene-based molecular dyad for single-component organic solar cells

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NMR Spectra:

Figure S1: $^1$H NMR (300 MHz) of TAT-Br in CDCl$_3$ at 20 °C.
**Figure S2**: $^1$H NMR (300 MHz) (top) and $^{13}$C NMR (76MHz) (bottom) of TAT-T in CDCl$_3$ at 20 °C.

**Figure S3**: $^1$H NMR (300 MHz) of TAT-T-CHO in CDCl$_3$ at 20 °C.
Figure S4: $^1$H NMR (300 MHz) (top) and $^{13}$C NMR (76MHz) (bottom) of TAT-$\sigma$-N$_3$ in CDCl$_3$ at 20 °C.
Figure S5: HRMS of TAT-\(\sigma\)-N\(_3\)
Figure S6: $^1$H NMR (300 MHz) (top) and $^{13}$C NMR (76MHz) (bottom) of TAT-σ C60 in CDCl3 at 20 °C.

Figure S7: HRMS of TAT-σ C60.
Figure S8: TAT-α-N₃ HOMO and LUMO and their corresponding energies calculated in vacuum (top) and including dichloromethane molecules as a polarizable continuum (bottom).

Figure S9: PC₆₁BM HOMO and LUMO and their corresponding energies calculated in vacuum (top) and including dichloromethane molecules as a polarizable continuum (bottom).
Electrochemical data:
Figure S10. Cyclic voltammograms of TAT-\(\sigma\)-N\(_3\) (red), TAT-\(\sigma\)-C\(_{60}\) (purple), and the PC\(_{61}\)BM (blue) in 0.1 M Bu\(_4\)NPF\(_6\)/CH\(_2\)Cl\(_2\), scan rate 100 mV s\(^{-1}\), Pt working and counter electrode.

Photovoltaic data:

Table S1. Photovoltaic data obtained from active layers processed with different solvents

| Processing solvent | Voc (V) | Jsc (mA cm\(^{-2}\)) | FF (%) | PCE (%) |
|--------------------|---------|-----------------------|--------|---------|
| CB                 | 0.41    | 1.77                  | 31.3   | 0.22    |
| CF                 | 0.81    | 1.80                  | 28.6   | 0.41    |
| MeTHF              | 0.04    | 1.40                  | 24.5   | 0.01    |
Figure S11. J−V characteristics measured under AM 1.5 simulated solar light under illumination (100 mW.cm⁻²) of the best devices processed with CB (bleu), CF (black) and MeTHF (red).

Atomic Force Microscopy:

Chlorobenzene (CB) processed active layers: RMS = 0.65 nm
Chloroform (CB) processed active layers: RMS = 0.65 nm

2-methyltetrahydrofuran (MeTHF) processed active layers: RMS = 21 nm

**Figure S12.** 2D and 3D surface topography images of the different active layers probed by atomic force microscopy