SUPPORTING INFORMATION

A BPTTF-based Self-Assembled Electrodonating Triangle capable of C_{60} binding

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General experimental methods – instruments.

Most of the spectroscopic data were obtained with the equipment facilities of the PIAM
(technical platform) at the University of Angers. The 500 \(^{1}H\), 202.5 \(^{31}P\) and 470.6 MHz
\(^{19}F\) NMR spectra were recorded at room temperature using perdeuterated solvents as
internal standards \(^{1}H\), external H\(_{3}\)PO\(_{4}\) solution \(^{31}P\) or CFCl\(_{3}\) \(^{19}F\). Mass spectra were
achieved on an ESI source spectrometer in CH\(_{3}\)CN at the Université de Rennes 1 (CRMPO).
Cyclic voltammetry experiments were carried out on a potentiostat-galvanostat with solvents
and electrolyte of electrochemical grades. CV experiments were carried out at 298K in a
conventional three-electrode cell equipped with a Pt disk working electrode (diameter: 1mm),
a Pt wire counter electrode, and a Ag wire reference electrode calibrated using an internal
ferrocen reference.
C₆₀ titration method.
A solution (2.5 mL) of triangle 2 (2.0 x 10⁻⁵ M) in CS₂ / CH₂Cl₂ (80 / 20) was placed in a UV-Vis cell equipped with a septum. Aliquots of the C₆₀ solution (2.0 x 10⁻³ M) in CS₂ / CH₂Cl₂ (80 / 20) were added into the working cell and into the reference cell containing 2.5 mL of CS₂ / CH₂Cl₂ (80 / 20). UV-Vis spectra were recorded at room temperature. To maintain a constant concentration the collected data were corrected from the dilution factor.

Materials. Methylene chloride was used as purchased. Compound 1¹ and complex $dpppPt(OTf)_2^2$ were synthesized as described in literature.

Synthesis.
Triangle 2: To a mixture of $dpppPt(OTf)_2$ (21.7 mg, 0.022 mmol) and compound 1 (10.0 mg, 0.022 mmol) was added CH₂Cl₂ (30 mL). The mixture was stirred for 5 days at room temperature. The insoluble square 3 was filtered and the resulting clear solution evaporated under an air flow to give 2 (19 mg, 60%) as a brown yellow solid. $^1$H NMR (500 MHz, acetone-d₆): δ 8.86 (d, $^3J = 5.8$ Hz, 12H), 7.88-7.79 (m, 24H) 7.48 (s, 12H), 7.46-7.39 (m, 36H), 7.31 (d, $^3J = 6.0$ Hz, 12H), 3.46 (s(b), 12H); $^{31}$P NMR (202.5 MHz, acetone-d₆): -12.98 (s); $^{19}$F NMR (470.6 MHz, acetone-d₆): -78.63 (s); ES-MS m/z (nature of the peak): 1862.5625 ([I-Ptdppp]₃.4TfO)²⁺; Anal. Calcd for C₁₄₅H₁₁₄F₁₂N₁₂O₁₂P₆S₂Pt₃ + 2CH₂Cl₂ : C, 42.64; H, 2.83; N, 4.01. Found: C, 42.58; H, 3.01; N, 4.11 %.

Figure S1. Analytical data for square 3
Figure S2. Front view of the energy-minimized structure (MM+) of square $3$ and triangle $2$ and their respective cavity size (the ligand $dppp$ was replaced with $dmpp$ (1,3-bis(dimethyl phosphine)propane) for a better readability).

Figure S3. Spectral changes in a UV-vis titration exp. of triangle $2$ (2.0 x $10^{-5}$ M) vs $C_{60}$ (2.0 x $10^{-3}$ M) at rt in CS$_2$ / CH$_2$Cl$_2$ (8 / 2). Inset: Benesi-Hildebrand curve from titration (log $K_a$ = 4.2; R = 0.995)

References.
