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_3PO_4 solution (^{31}P) or $CFCl_3$ (^{19}F). Mass spectra were achieved on a ESI source spectrometer in CH_3CN 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.

C_{60} titration method.

A solution (2.5 mL) of triangle **2** (2.0 x 10^{-5} M) in CS_2 / CH_2Cl_2 (80 / 20) was placed in a UV-Vis cell equipped with a septum. Aliquots of the C_{60} solution (2.0 x 10^{-3} M) in CS_2 / CH_2Cl_2 (80 / 20) were added into the working cell and into the reference cell containing 2.5mL of CS_2 / CH_2Cl_2 (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 **1**[1] and complex *dppp*Pt$(OTf)_2$[2] were synthesized as described in literature.

Synthesis.

Triangle 2: To a mixture of *dppp*Pt$(OTf)_2$ (21.7 mg, 0.022 mmol) and compound **1** (10.0 mg, 0.022 mmol) was added CH_2Cl_2 (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-d_6): 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-d_6): -12.98 (s); ^{19}F NMR (470.6 MHz, acetone-d_6): -78.63 (s); ES-MS m/z (nature of the peak): 1862.5625 ([**1**-Ptdppp)$_3$.4TfO$^-$]$^{2+}$; Anal. Calcd for $C_{145}H_{114}F_{12}N_{12}O_{12}P_6S_2Pt_3$ + $2CH_2Cl_2$: C, 42.64; H, 2.83; N, 4.01. Found: C, 42.58; H, 3.01; N, 4.11 %.

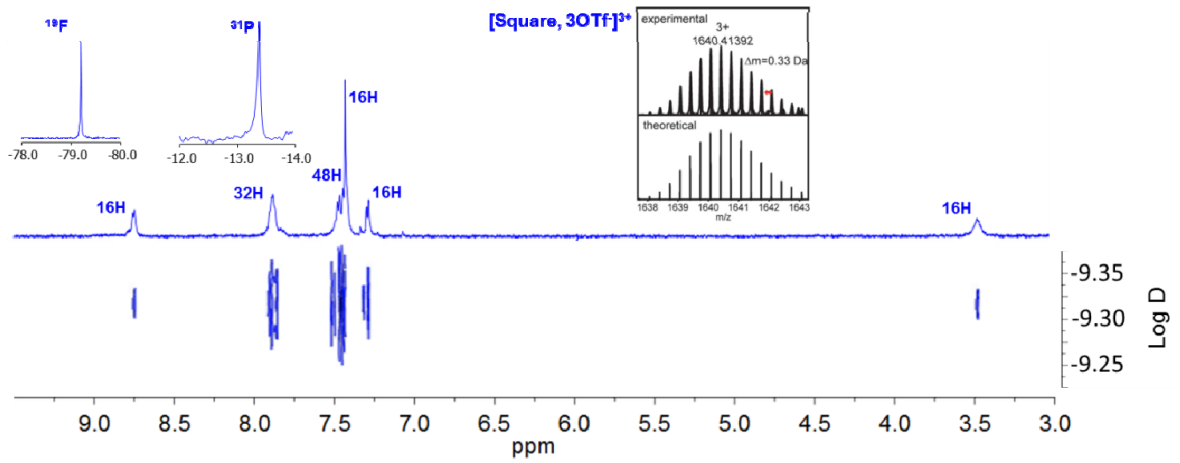

Figure S1. Analytical data for square **3**

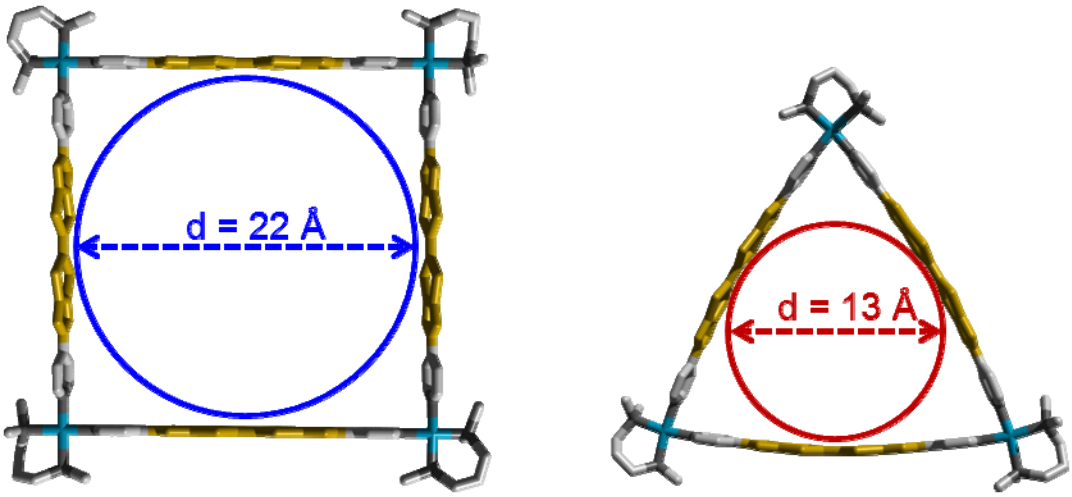

Figure S2. Front view of the energy-minimized structure (MM+) of square **3** and triangle **2** and their respective cavity size (the ligand *dppp* was replaced with *dmpp* (1,3-bis(dimethyl phosphine)propane) for a better readability).

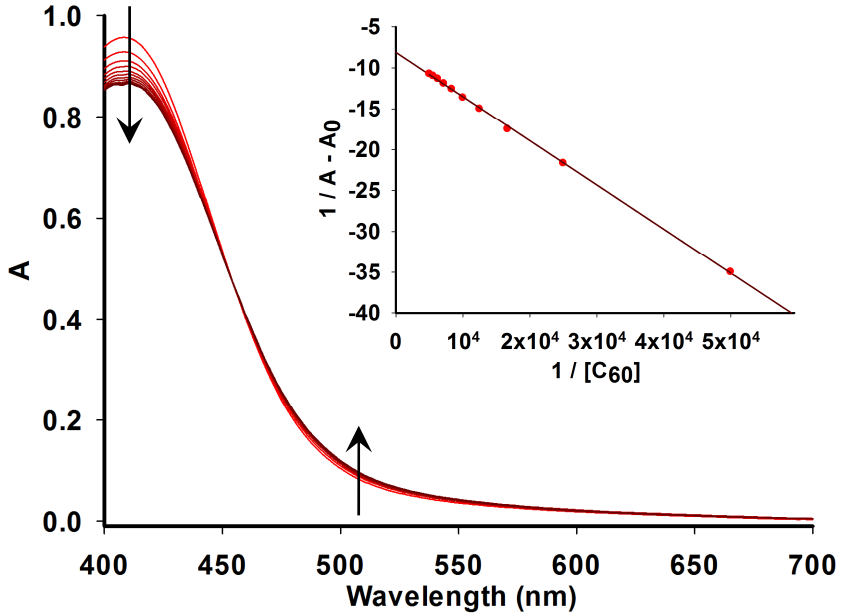

Figure S3. Spectral changes in a UV-vis titration exp. of triangle **2** (2.0 x 10^{-5} M) vs C_{60} (2.0 x 10^{-3} M) at rt in CS_2 / CH_2Cl_2 (8 / 2). Inset: Benesi-Hildebrand curve from titration (log K_a = 4.2; R = 0.995)

References.

1. J. Y. Balandier, M. Chas, S. Goeb, P. I. Dron, D. Rondeau, A. Belyasmine, N. Gallego and M. Sallé, *New J. Chem.* 2011, **35**, 165.
2. P. J. Stang, D.H. Cao, S. Saito and A. M. Arif, *J. Am. Chem. Soc.* 1995, **117**, 6273.