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Electronic Supplementary Information

High Yield Synthesis of a New Fullerene Linker and Its Use in the Formation of Linear Coordination Polymer by Silver Complexation

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EXPERIMENTAL SECTION

Materials and Methods. All chemicals were obtained from commercial sources and used without further purification. The NMR spectra were recorded using a JEOL 600 NMR spectrometer.MALDI−TOF MS was conducted on a Bruker Microflex LRF mass spectrometer. The UV−vis−NIR spectrum was recorded using a Cary 5000 UV−vis−NIR spectrophotometer.

Synthesis of *Trans*-1 Hexakis-Adduct 4. To a solution of 100.0 mg (0.073 mmol) of **3**, 53.7 mg (0.162 mmol) of CBr_4, and 27.2 mg (0.162 mmol) of 4, 5-diazafluorene in 50 mL of CH_2Cl_2 was added 44.9 mg (0.294 mmol) of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU). The reaction mixture was allowed to stir at room temperature for 3h. The solvent was then removed under reduced pressure and the mixture was purified by Prep-TLC to get light yellow solid (114 mg, 91% yield). Data for **4**: ^{1}H NMR (125 MHz, $CDCl_3$, TMS): δ = 8.80 (d, 4H, J = 4.8 Hz), 8.69 (d, 4H, J = 6.4 Hz), 7.41 (m, 4H), 4.45 (dd, 8H, J_{12} = 7.2 Hz, J_{13} = 14.4 Hz), 4.21 (dd, 1H, J_{12} = 7.2 Hz, J_{13} = 14.4 Hz), 1.41 (t, 12H, J = 7.2 Hz), 1.23 ppm (t, 12H, J = 7.2 Hz). ^{13}C NMR (600 MHz, $CDCl_3$): δ = 164.15, 163.61, 150.04, 146.10, 145.96, 142.71, 141.02, 138.24, 133.14, 123.39, 74.64, 69.64, 69.30, 63.50, 63.15, 14.23, 14.11 ppm. MALDI-TOF-MS: (positive ionization mode 9-nitroanthracene as matrix): $[M+H]^+$ 1685.391. UV-vis (CH_2Cl_2): λ = 285 nm, 318 nm, 340 nm, 395 nm.

X-ray Crystallography and Data Collection of 4a. Crystal data for **4a**, **4**•2Ag(triflate)•5toluene. Crystals were grown by a slow diffusion of a methanol solution of Ag(triflate) into a solution of **4** in dichloromethane followed by diffusion of toluene into the resulting solution. $C_{147}H_{92}Ag_2F_6N_4O_{22}S_2$, fw 2660.13, yellow-green lamellar crystals, 0.048 x 0.032 x 0.0084 mm, triclinic, space group *P*-1, a = 13.563(4), b = 14.330(3), c = 15.134(3), α = 72.722(11), β = 76.995(18), γ = 88.831(14), V = 2733.2(11) Å, λ = 0.77490 Å, Z = 1, ρ_{calcd} = 1.616 Mg m^{-3}; μ = 0.609mm^{-1}, T = 100(2) K; ALS Beamline 11.3.1 Bruker Apex II CCD detector; ω scans, $2\Theta_{max}$=58.1; 45444 reflections collected; 11158 independent (R_{int} = 0.0380) included in the refinement; min/max transmission=0.97/0.99 (SADABS-2008);[1]

Direct methods solution (SHELXS97); full matrix least squares based on F^2(SHELXL97);[2] R = 0.0390; wR = 0.0955 for all data; conventional R_1 = 0.0349 computed for the 10100 observed data ($I > 2\sigma(I)$) with 864 parameters and 15 restraints.

X-ray Crystallography and Data Collection of 4b. Crystal data for **4b**, **4**•2Ag(toluene)$_2$•2(tetrafluoroborate)•dichloromethane•toluene. Crystals were grown by slow diffusion of $AgBF_4$ in methanol into a solution of **4** in dichloromethane followed by diffusion of toluene into the resulting solution. $C_{146}H_{94}Ag_2B_2Cl_2F_8N_4O_{16}$, fw 2620.51, yellow needle, 0.036 x 0.127 x 0.290 mm, triclinic, space group *P*1, a = 11.0646(9), b = 15.0722(11), c = 17.0040(12), α = 95.111(4), β = 104.041(4), γ = 94.393(4)), V = 2714.3(4) Å, λ = 0.77490 Å, Z = 1, ρ_{calcd} = 1.603 Mg m^{-3}; μ = 0.502mm^{-1}, T = 100(2) K; ALS Beamline 11.3.1 Bruker Apex II CCD detector; ω scans, $2\Theta_{max}$ = 75.46; 92741 reflections collected; 92741 independent (R_{int} = 0.0405) included in the refinement; min/max transmission = 0.87/0.98 (SADABS-2008);[1] direct methods solution (SHELXS97); full matrix least squares based on F^2(SHELXL97);[2] R = 0.0553; wR = 0.1421 for all data; conventional R_1 = 0.0512 computed for the 38850 observed data ($I > 2\sigma(I)$) with 1612 parameters and 9 restraints; the value of the Flack parameter refined to 0.307(8).

1. Sheldrick, G. M. *University of Göttingen, Germany.* 2001

2**.** Sheldrick, G. M. *Acta Crystallogr. Sect. A.* 2008, **64**, 112.