Novel Soluble and Thermal-stable Fullerene Dyad Containing Perylene

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Supplementary Information

The synthesis of 1, 6, 7, 12- tetra(4-tert-butylphenoxy)-3, 4, 9, 10-perylene tetracarboxylic dianhydride (2). To a solution of KOH (15.7 g, 280 mmol) and isopropanol (200 mL) in a three-necked round bottomed flask equipped with a mechanical stirrer, a nitrogen inlet and a condenser, was added N, N′-dibutyl-1, 6, 7, 12-tetra(4-tert-butylphenoxy)-3, 4, 9, 10-perylenetetracarboxylic diimide (5 g, 4 mmol). The mixture was refluxed under argon for 24 hours. After cooling to room temperature, the reaction mixture was neutralized with 8 vol. % HCl solution. The precipitate appeared was washed with water and dried under vacuum at 60 °C. The product was recrystallized from CH_2Cl_2 / MeOH gave 3.70 g (80 %) of compound as red powers. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.32 (s, 4 H), 7.21 (d, J = 8.23Hz, 8 H), 6.81 (d, J = 8.39 Hz, 8 H), 1.32 (s, 36 H). Anal. Calcd. for

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$C_{64}H_{56}O_{10}$ (Mw, 985.14): C, 78.03; H, 5.73. Found: C, 78.27; H, 5.69.

The synthesis of N-(n-butyl)-1, 6, 7, 12-tetra(4-tert-butylphenoxy)-3, 4, 9, 10-perylenetetracarboxylic monoimide (3). A solution of 1, 6, 7, 12-tetra(4-tert-butylphenoxy)-3, 4, 9, 10-perylenetetracarboxylic dianhydride (3.62 g, 4.6 mmol) and n-butylamine (0.41 mL, 3.92 mmol) in toluene (80 mL) was refluxed for 20h. The solvent was evaporated and propionic acid (100 mL) was added to the residue. A slow stream of ammonia was bubbled into the reaction mixture until its weight was increased by 10 g. The reaction mixture was then refluxed for another 14h. After cooling to room temperature, the crude product was precipitated from the red solution by addition of water (100 mL), washed with water and dried. The crude compound was separated by column chromatography on silica gel (CH_2Cl_2) to give the pure product (0.80 g, 35 %). ^{1}H NMR (500MHz, $CDCl_3$): δ 8.42 (s, 1H), 8.22 (s, 4 H), 7.24 (d, J = 8.25 Hz, 8 H), 6.82 (d, J = 8.37 Hz, 8 H), 4.11 (t, 2 H), 1.65 (m, 2 H), 1.40 (m, 2 H), 1.29 (s, 36 H), 0.93 (t, 3 H). Anal. Calcd. for $C_{68}H_{66}N_2O_8$ (Mw, 1039.27): C, 78.59; H, 6.40; N, 2.69. Found: C, 78.67; H, 6.32; N, 2.87.

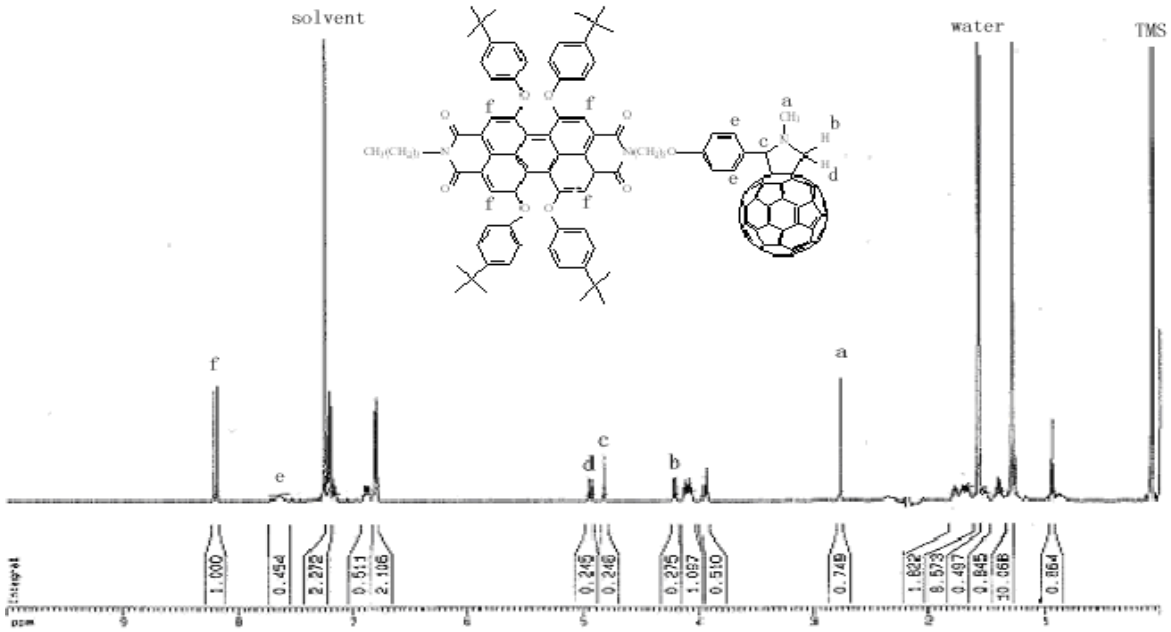


Fig. S1 The H NMR spectra of **C_{60}-P1**

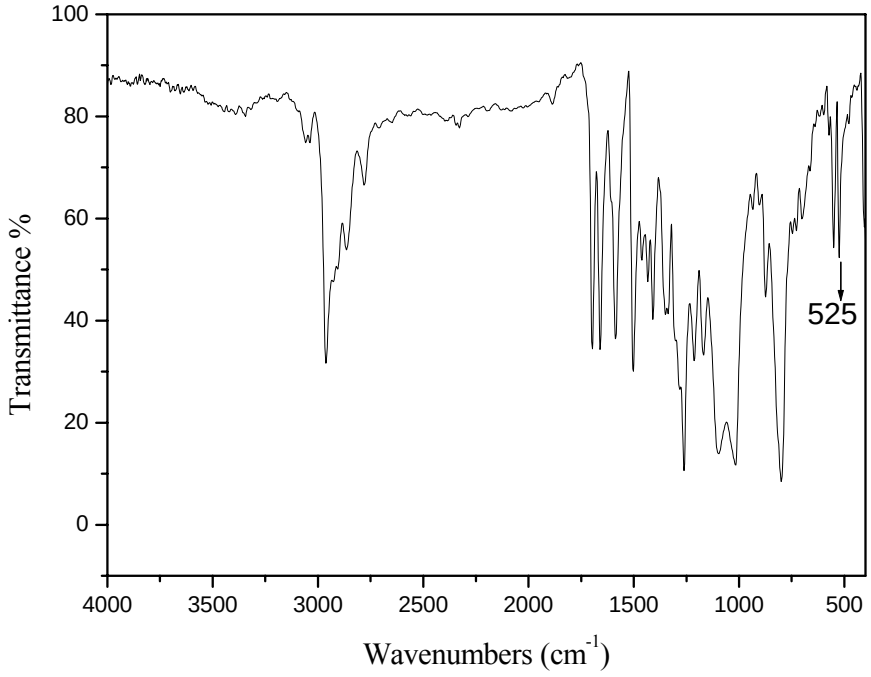


Fig. S2 The IR spectra of **C_{60}-P1**

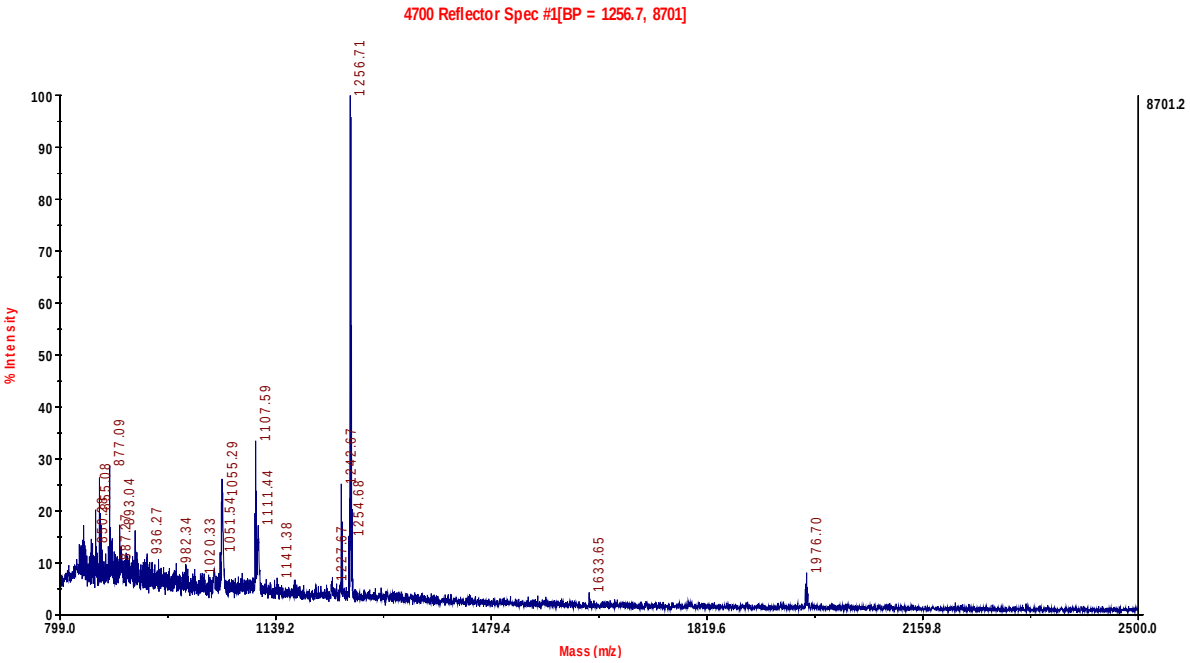


Fig. S3 The MS spectra of **C_{60}-P1**

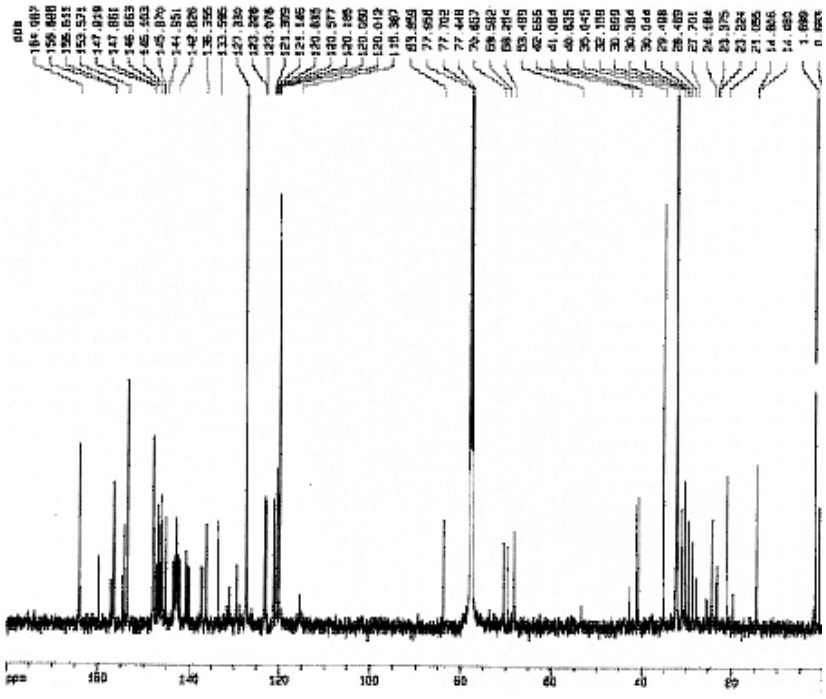


Fig. S4 The ^{13}C NMR spectra of **C_{60}-P1**

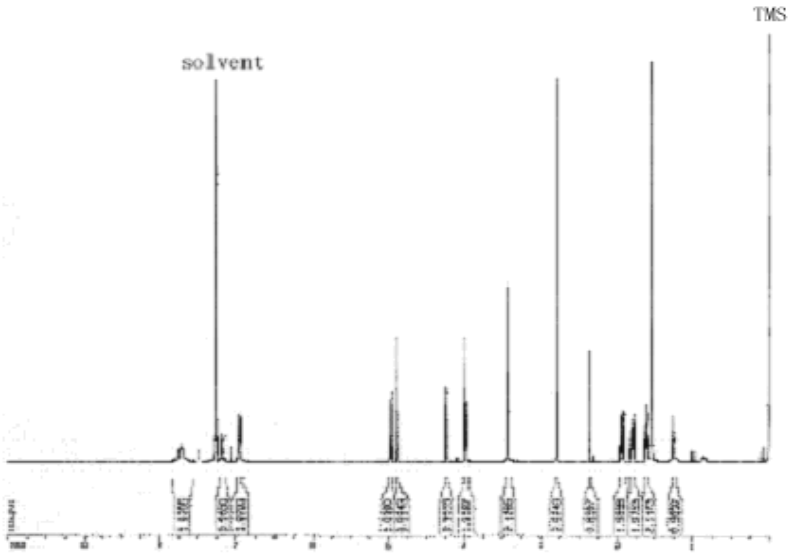
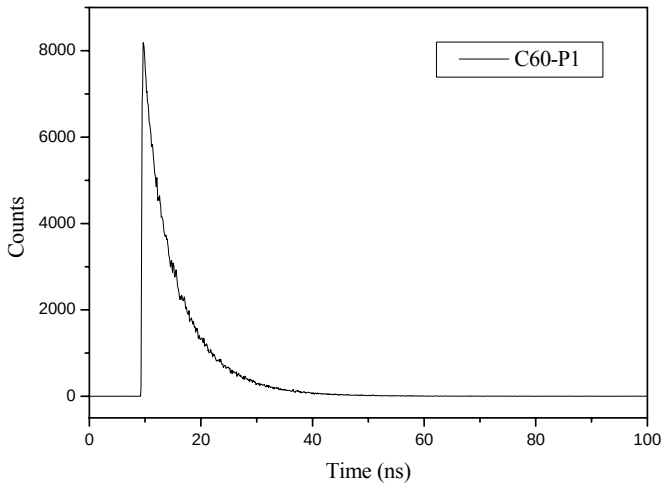
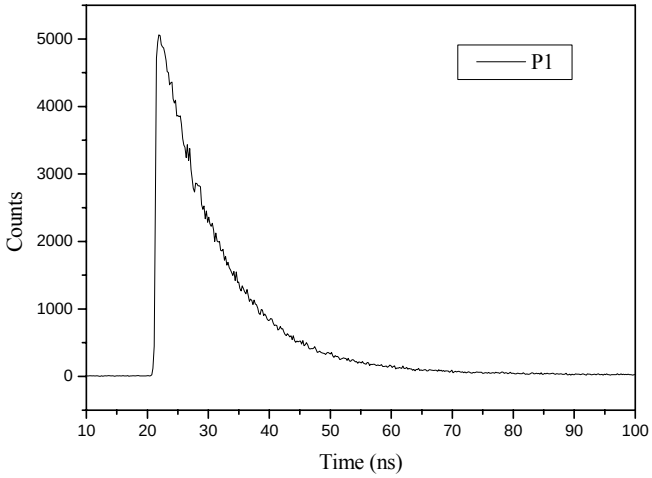


Fig. S5 The ^{1}H NMR spectra of **FP**





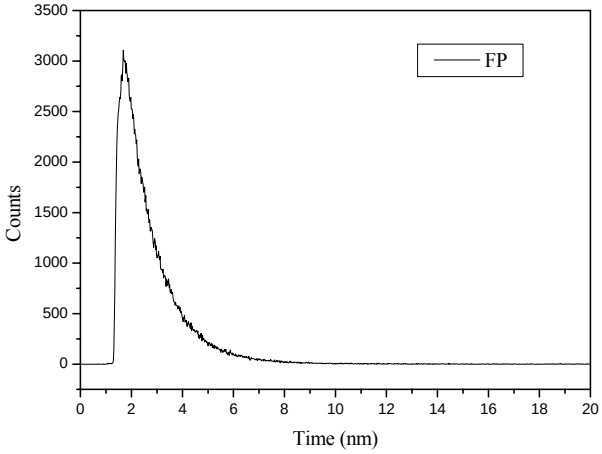


Fig. S6 Emission lifetimes of **C_{60}-P1, P1**, and **FP** in CH_2Cl_2 (1×10^{-5} mol L^{-1}) excited at 370 nm Fluorescence lifetimes are measured by Time-Correlated Single Photon Counting using an Edinburgh Instruments LifeSpec-PS spectrometer. The LifeSpec-PS comprises a 371 nm picosecond laser (PicoQuant PDL 800B) operated at 2.5 MHz and a filter-cooled Hammamatsu micro-channel plate photomultiplier (R3809U-50). Lifetimes were determined from the data using the Edinburgh Instruments software package.