A New Fullerene Complexation Ligand: N-Pyridylfulleropyrrolidine

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Supporting Information

	Page
¹ H NMR and mass spectrum of compound 1	S2
¹ H NMR spectrum of complex 1 -ZnTPP	S3
¹ H NMR and mass spectrum of compound 3	S4
¹ H NMR and mass spectrum of compound 4	S5
Figure A. Center-to-center distances for 1 -ZnTPP vs. 2 -ZnTPP	S6
Figure B1. UV spectra of compounds 1 , 2 , 3 and 4	S6
Figure B2. UV spectrum of ZnTPP and its complex	S7
Figure C. Spartan calculation results of 1 , 2 , 3 and 4	S7
Figure D. HOMOs and LUMOs of free base 1 vs. its salt 3	S8
Figure E. HOMOs and LUMOs of free base 2 vs. its salt 4	S9
Figure F. Cyclic voltammograms of 1 , 2 , 3 , 4 in CH ₂ Cl ₂	S10
Figure G. Cyclic voltammogram of compound 3 in acetonitrile	S11
Figure H. Numbered ortep figure for X-ray structure of compound 1 -ZnTPP (see CIF tables for data)	S12
Figure I. Crystal packing diagram for 1 -ZnTPP	S13

^1H NMR spectrum of compound **1**

Mass spectrum of compound **1**

^1H NMR spectrum of complex **1-ZnTPP**

^1H NMR spectrum of compound **3**

Mass spectrum of compound **3**

^1H NMR spectrum of compound **4**

Mass spectrum of compound **4**

Figure A. Center-to-center distances for **1**-ZnTPP vs. **2**-ZnTPP

Figure B1. UV-vis spectra of compounds **1**, **2**, **3** (salt of **1**) and **4** (salt of **2**) in CH_2Cl_2

Figure B2. UV-vis spectra of ZnTPP and its complex

Figure C. a: Free base compound **1**. **b:** Salt of compound **1**. **c:** Free base compound **2**. **d:** Salt of compound **2**. Protonation of the N-atom of the pyridine leads to greater charge separation in the case of compound **1** than compound **2**

Figure D. HOMOs and LUMOs of free base **1** vs. its salt **3**

Figure E. HOMOs and LUMOs of free base **2** vs. its salt **4**

Figure F. Cyclic voltammograms of **1**, **2**, **3**, **4** in CH₂Cl₂. The irreversible reduction peak at -1.8 V, which is not observed for compound **3** likely corresponds to the irreversible reduction of the pyridinium group of **4**. The C₆₀-based waves are reversible when the scan potential is switched at -1.67 V (red curve).

Figure G. Cyclic voltammogram of compound **3** in acetonitrile. The couple at -2.22 V can be attributed to the reduction of the pyridinium group in compound **3** since the potential value is very close to that (-1.77 V vs. Ag/Ag/Cl or -2.2 V vs. Fc/Fc⁺) for the model compound reported by Huenig et al [Huenig, S., Ort, B., Wenner, H., *Liebigs Annalen der Chemie*, **1985**, 751]. Alternatively, the couple at -2.37 V could be attributed to reduction of the pyridinium attached to the pyrrolidine in compound **3** and the couple at -2.22 V could correspond to the fourth C₆₀-based one-electron reduction.

Figure H. Numbered ortep figure for X-ray structure of compound **1**-ZnTPP
(see CIF tables for data)

Figure I. Crystal packing diagram for **1-ZnTPP**