Supporting Information

Electronic Properties and ^{13}C NMR Structural Study of $Y_3N@C_{88}$

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1. **Information for Figure 2: The experimental ^{13}C NMR shifts of $Y_3N@D_2$-C_{88} (22 lines)** in CS_2 with 10 mg $Cr(acac)_3$ relaxant, acetone-d_6 lock) after 64,000 scan at 25 ºC. The chemical shifts for the 22 lines are at δ: 149.36, 148.89, 146.44, 146.21, 145.77, 144.44, 143.92, 143.64, 141.89,. 140.07, 139.69 (double intensity), 139.59, 139.10 (double intensity), 138.34, 137.88, 136.14, 135.19, 133.76, 133.65, 132.06, 131.99 ppm. 2. **The computational ^{13}C NMR chemical shifts of $Y_3N@D_2$(35)-C_{88} (22 lines):** 151.66, 147.21, 146.76, 146.24, 144.00, 143.89, 143.18, 142.14, 142.10, 141.66, 141.27, 140.53, 140.02, 139.76, 139.29, 139.27, 137.99, 137.43, 136.25, 135.66, 135.54, 131.94 ppm.

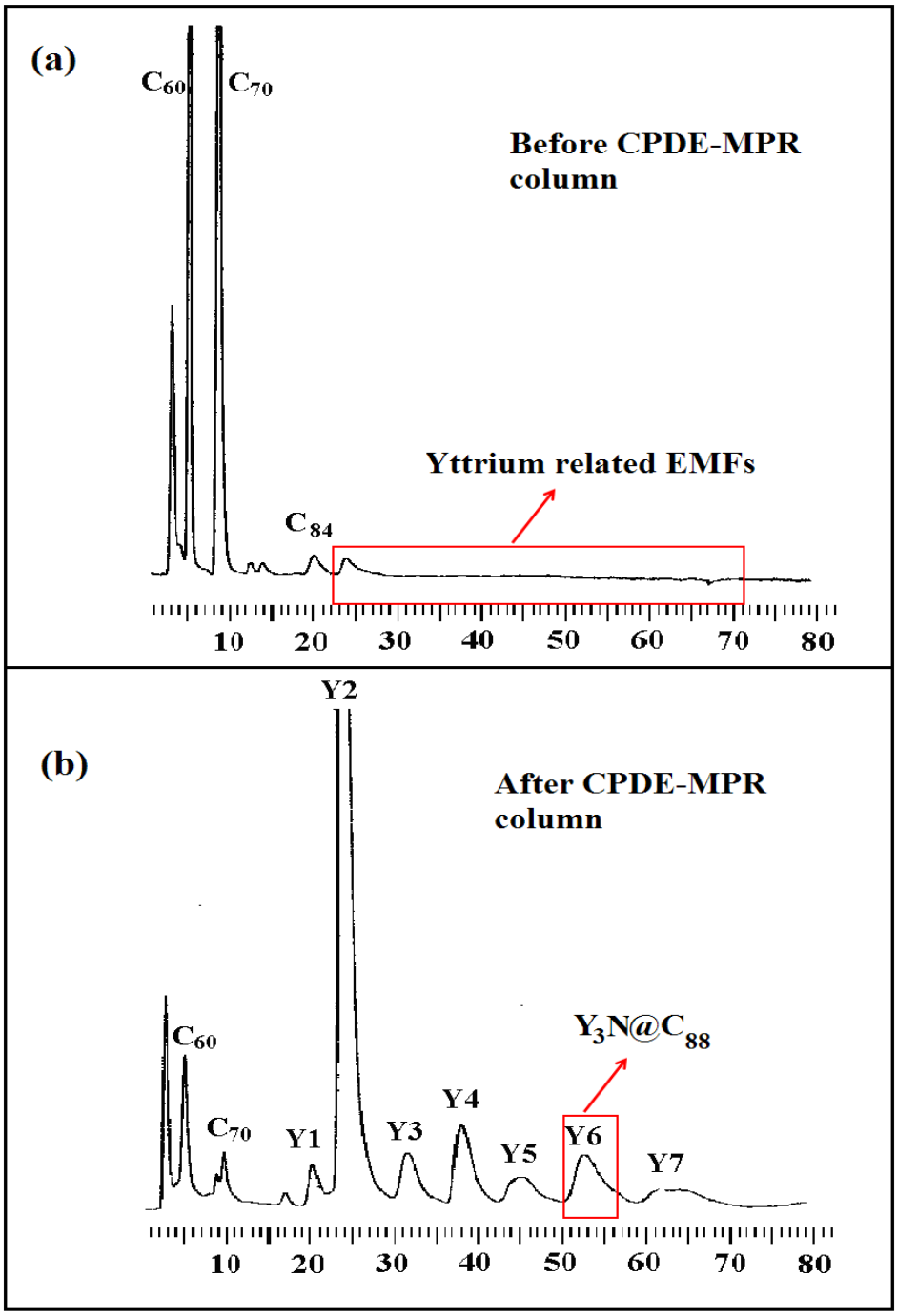

Figure S1. (a) HPLC chromatogram of the toluene extract from the raw soot (b) HPLC chromatogram of the eluent from CPDE-MPR column (Both chromatogram on a 4.6 × 250 mm 5PBB column; λ=390 nm; flow rate 2.0 mL/min; toluene as eluent; 25 ºC)

Table S1. The component and yield of each Yttrium fractions

Fraction	Main component	Yield (mg)*
Y1	$Y_2@C_{79}N$	0.005
Y2	$Y_3N@C_{80}$	2
Y3	$Y_3N@C_{82}$	0.05
Y4	$Y_3N@C_{84}$	0.1
Y5	$Y_3N@C_{86}$	0.01
Y6	$Y_3N@C_{88}$	0.01
Y7	Y_2C_{94}	0.01

- (the estimated yield is based on "burning" 3, 6 x 1 inch rods. However, 50-100 rods were burned to obtain the sample utilized in this study.)

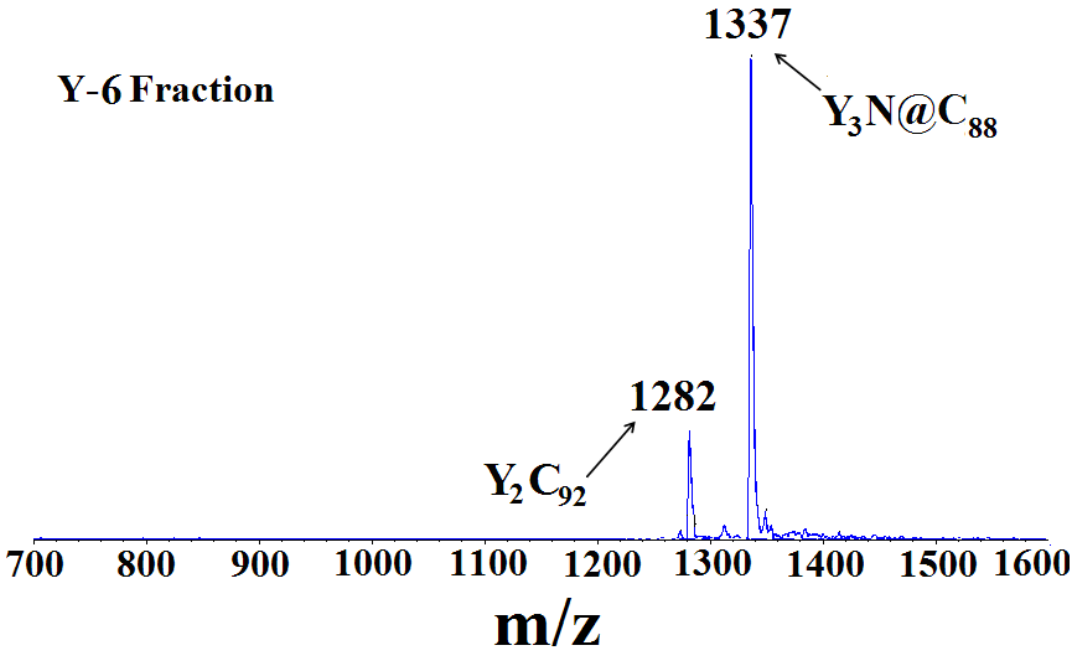

Figure S2. The LD-TOF mass spectrum of Y-6 fraction with positive ionization.

Figure S3. The LD-TOF mass spectrum of Gd-6 fraction ($Gd_3N@C_{88}$) with positive ionization.