Supporting Information

Self-Assembly of Molecular Nanoball: Design, Synthesis and Characterization

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General Experimental Methods

^1H NMR and ^{13}C spectra were recorded in a 400 – MHz machine. Thermogravimetric analyses were performed using a TGA attached to a mass spectrometer under a flow of nitrogen (30 mL min^{-1}). The sample (particle size 50-200 mesh) was heated at a rate of $10\text{ }^{\circ}\text{C min}^{-1}$ with inert alumina as a reference. ^1H chemical shifts are reported relative to the residual protons of deuterated dimethylsulfoxide (δ 2.5 ppm). IR spectra were recorded in KBr pellets. The mass spectra were obtained under electrospray ionization using a dimethylsulfoxide and acetonitrile (1:2) solution of the complexes **2a** and **2b**.

Figure-S1: ^1H NMR of **1b** and **2b**.

Figure S2: ^{13}C NMR of 1a.

Figure S3: ^{13}C NMR of 2a.

Figure S4: ^{13}C NMR of 1b.

Figure S5: ^{13}C NMR of 2b.

Figure S6: Hetero-COSY (^{13}C - ^1H) of the complex **2b**. Two separate cross peaks (encircled) are due to the H_c protons.

Figure-S7: TGA plot of **2a** between 25-500 °C.

Figure S8: Absorption spectra of cage **2a** (0.5 μ M) and ligand **1a** (4 μ M).

Figure S9: NMR of the mixture of **2a** and 5 equiv **3** after 2h of stirring (bottom). Peaks due to the inclusion of **3** are shown by *. Pure inclusion complex (**2a·3**)¹³⁺ after isolating by acetone addition(top).