Electronic Supplementary Information for

Switching a molecular shuttle on and off: Simple, pH-controlled pseudorotaxanes based on cucurbit[7]uril

Vladimir Sindelar, Serena Silvi and Angel E. Kaifer*

Center for Supramolecular Science and Department of Chemistry, University of Miami, Coral Gables, FL 33124-0431, U.S.A.

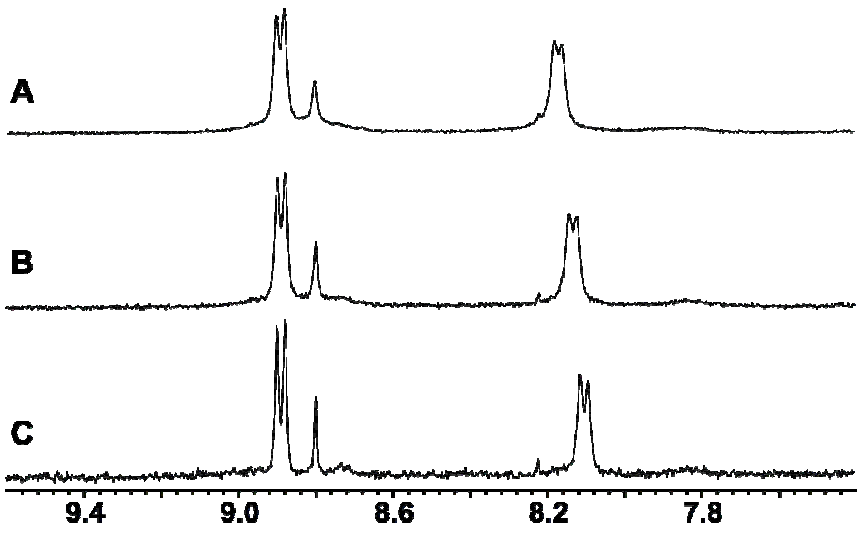

Figure S1. ^{1}H NMR partial spectra (300 MHz, 0.1 M NaCl/D_2O) of $\mathbf{1}^{2+}$ in the presence of 1.2 equiv CB7 at (A) 5.52 mM, (B) 1.83 mM, and (C) 0.92 mM $\mathbf{1}^{2+}$.

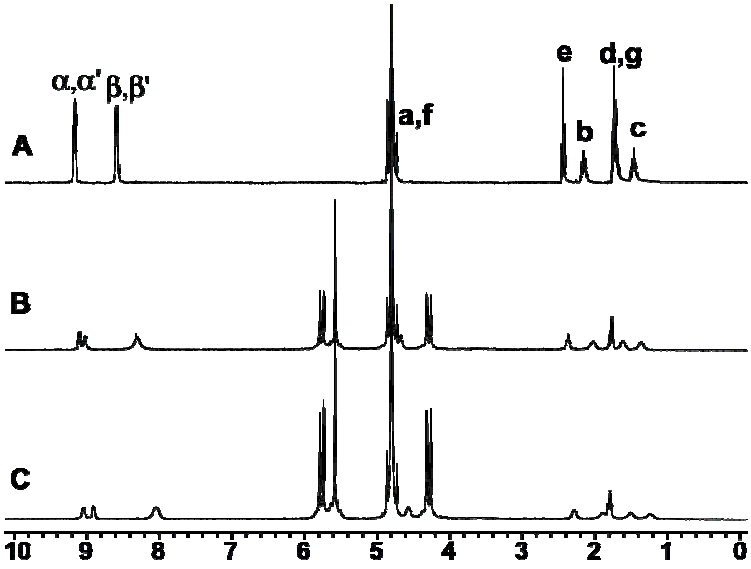

Figure S2. ^{1}H NMR spectra (300 MHz, 0.1 M NaCl/D_2O) of guest $\mathbf{3}^{2+}$ (A) in the absence and in the presence of (B) 0.5 equiv CB7 at (C) 1.1 equiv CB7.

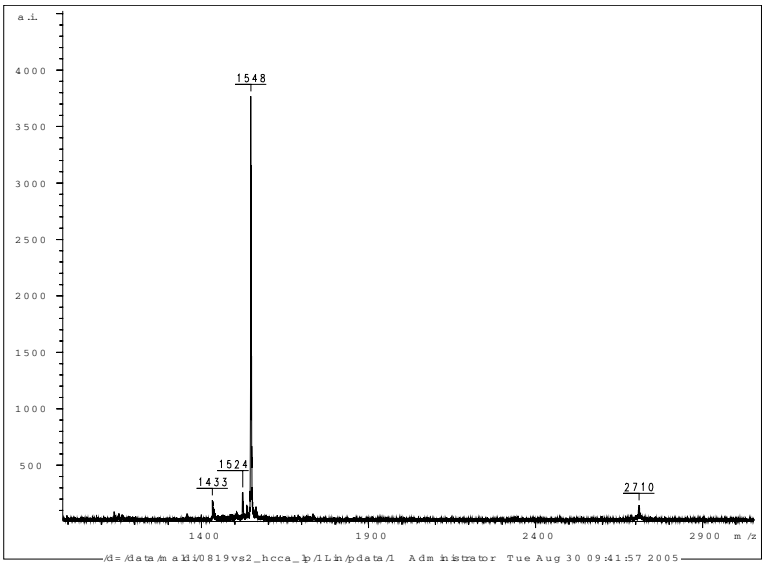

Figure S3. MALDI-TOF MS spectra of a solution containing $\mathbf{1}^{2+}$ (1 equiv) and CB7 (2.5 equiv) in water recorded from an α-cyano-4-hydroxy-cinnamic acid solid matrix. The peaks at 1,548 and 2,710 were assigned to $[CB7\bullet\mathbf{1}]^{+}$ and $[(CB7)_2\bullet\mathbf{1}]^{+}$, respectively.

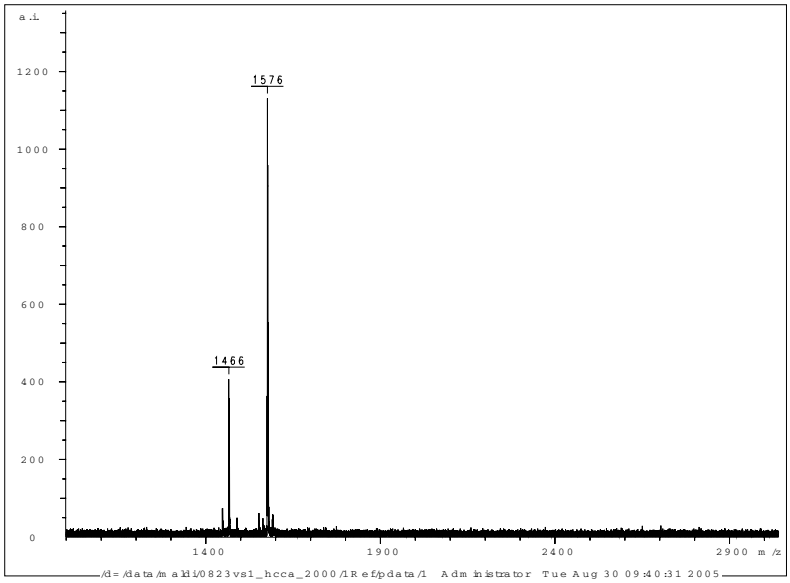

Figure S4. MALDI-TOF MS spectra of a solution containing $\mathbf{2}^{2+}$ (1 equiv) and CB7 (1 equiv) in water recorded from an α-cyano-4-hydroxy-cinnamic acid solid matrix. The peak at 1,576 was assigned to $[CB7\bullet\mathbf{2}]^{+}$.

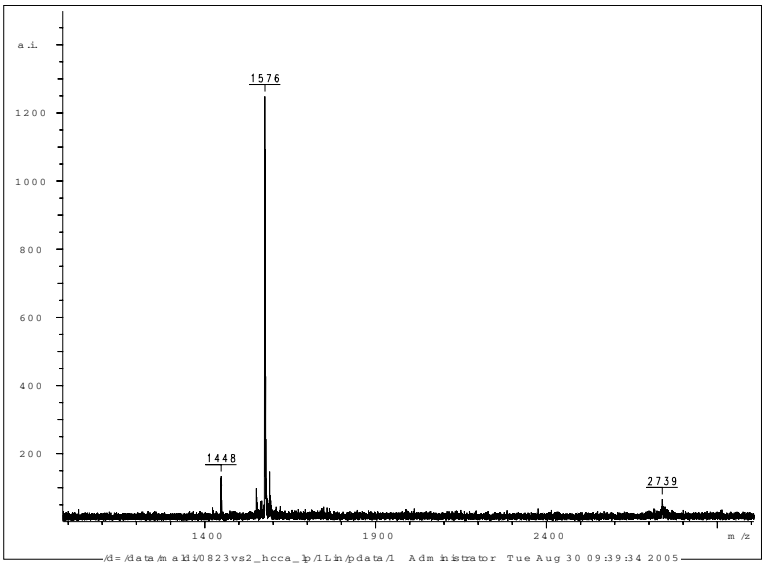

Figure S5. MALDI-TOF MS spectra of solution containing $\mathbf{2}^{2+}$ (1 equiv) and CB7 (2.5 equiv) in water recorded from an α-cyano-4-hydroxy-cinnamic acid matrix. The peaks at 1,576 and 2,739 were assigned to $[CB7\bullet\mathbf{2}]^{+}$ and $[(CB7)_2\bullet\mathbf{2}]^{+}$, respectively.

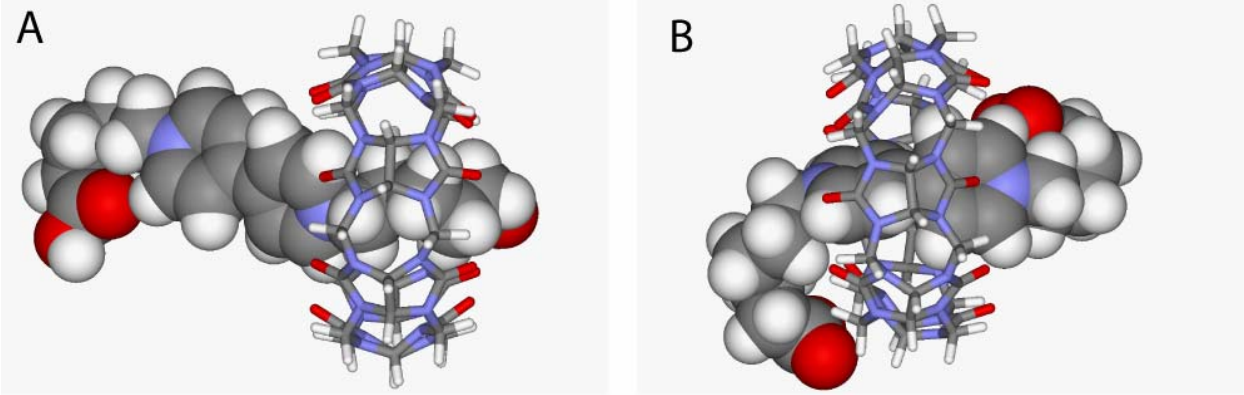

Figure S6. Energy minimized structures as calculated with the semi-empirical AM1 method for the (A) protonated (CB7•$\mathbf{1}^{2+}$) and (B) deprotonated (CB7•**1**) forms of the complex.