A Host-Induced Intramolecular Charge-Transfer Complex and Light-Driven Radical Cation Formation of A Molecular Triad with Cucurbit[8]uril

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I. ^{1}H NMR of triad 1 with different equiv CB[8]

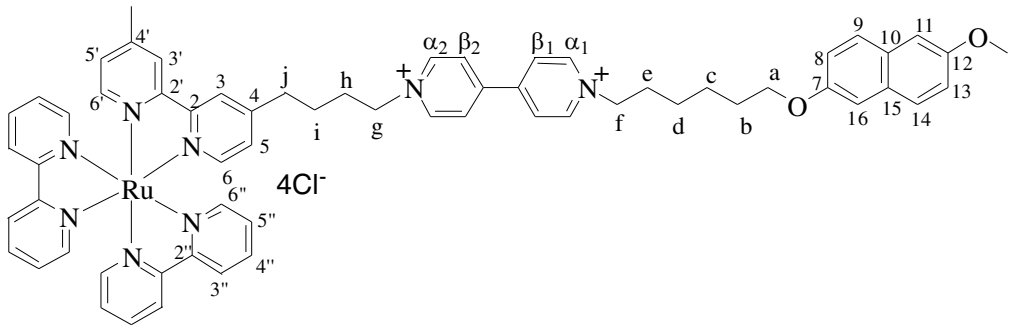


Chart S1. The structure of triad **1** and the labeling scheme for the ^{1}H NMR resonances

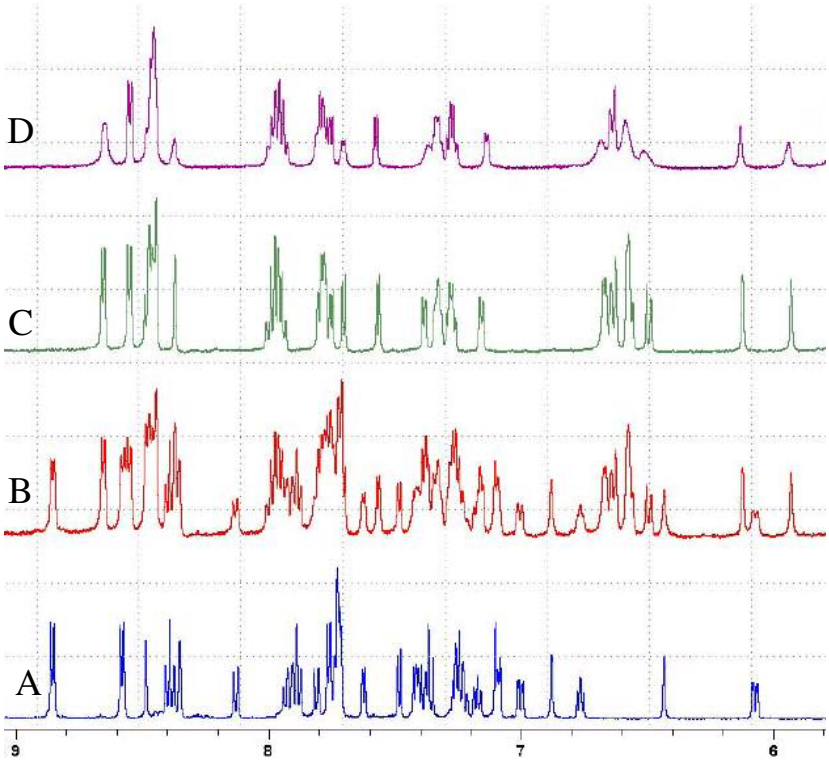


Figure S1. ^{1}H NMR spectra (500 MHz, D_2O) of triad **1** in the absence (A), in the presence of 0.5 equiv.(B), 1 equiv. (C), 2 equiv. of CB[8](D).

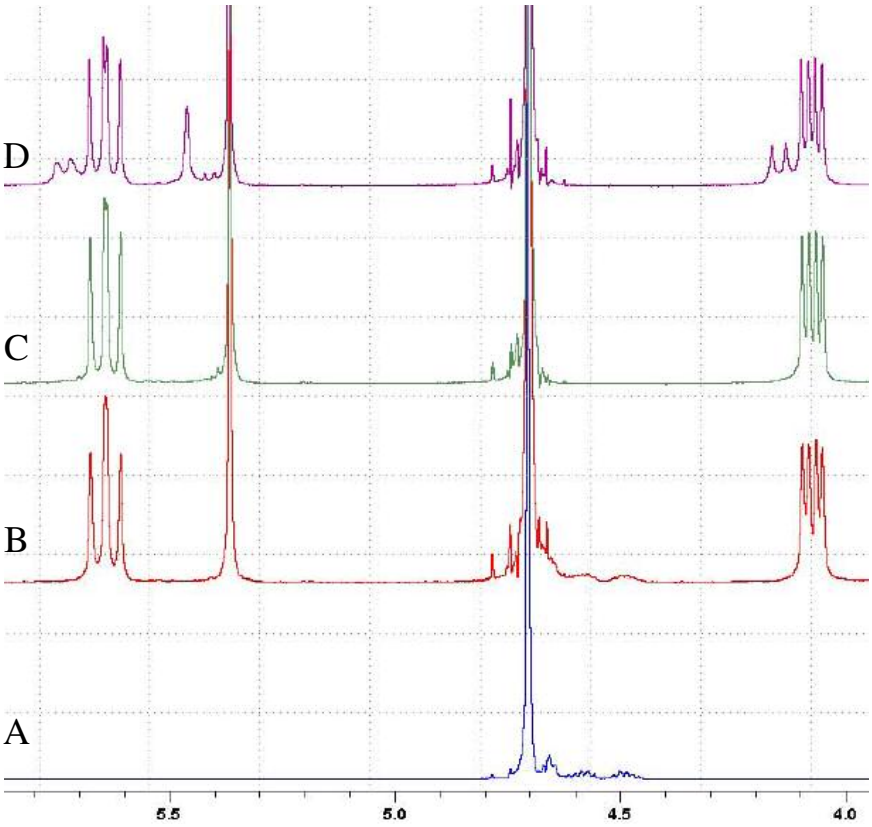


Figure S2. ^{1}H NMR spectra (500 MHz, D_2O) of triad **1** in the absence (A), in the presence of 0.5 equiv.(B), 1 equiv. (C), 2 equiv. of CB[8](D).

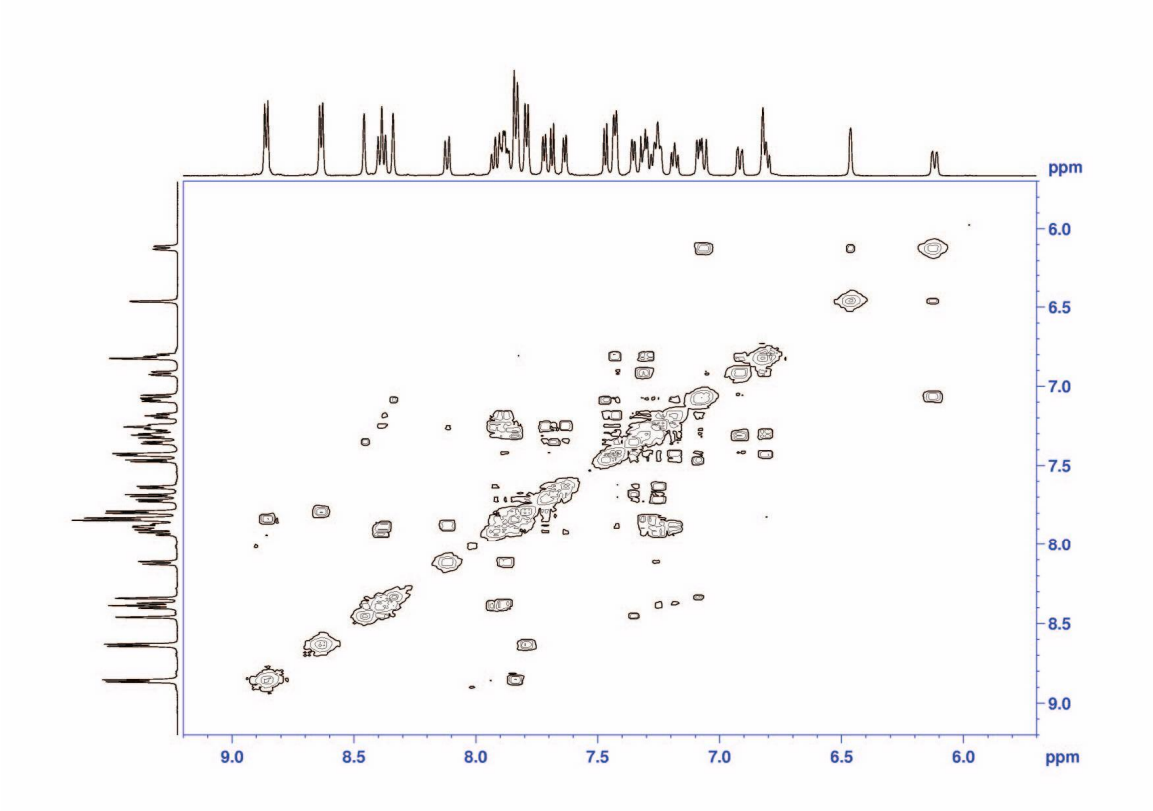


Figure S3. COSYGPSW spectra (500 MHz, D_2O) of triad **1** in the absence of CB[8], aromatic top region. See figure 2 for peak assignment.

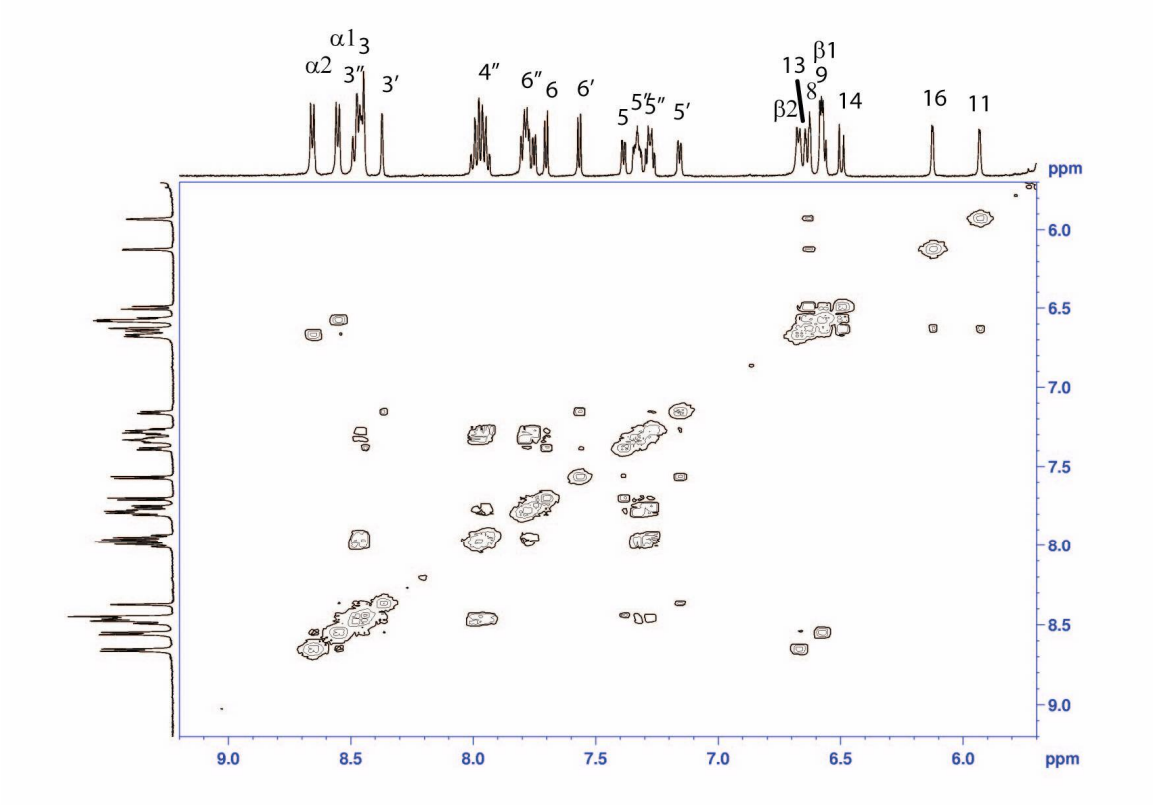
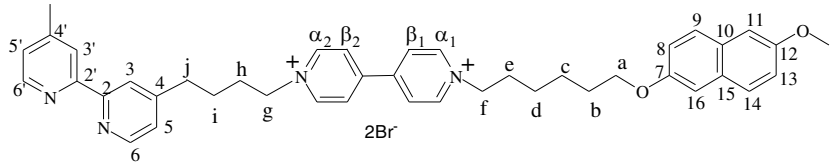


Figure S4. COSYGPSW spectra (500 MHz, D_2O) of triad **1** in the presence of 1 equivalent CB[8], aromatic top region.

II. ^{1}H NMR of ligand 2 with equivalent of CB[8]



ligand 2

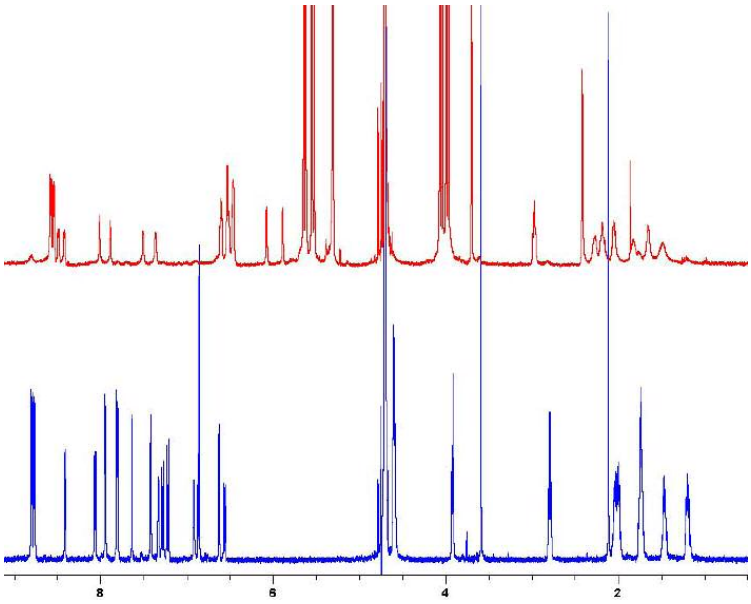


Figure S5. ^{1}H NMR spectra (500 MHz, D_2O) of ligand **2** in the absence (bottom), in the presence of 1 equiv (above) CB[8].

III. The electrochemical behavior of triad 1 with CB[8]

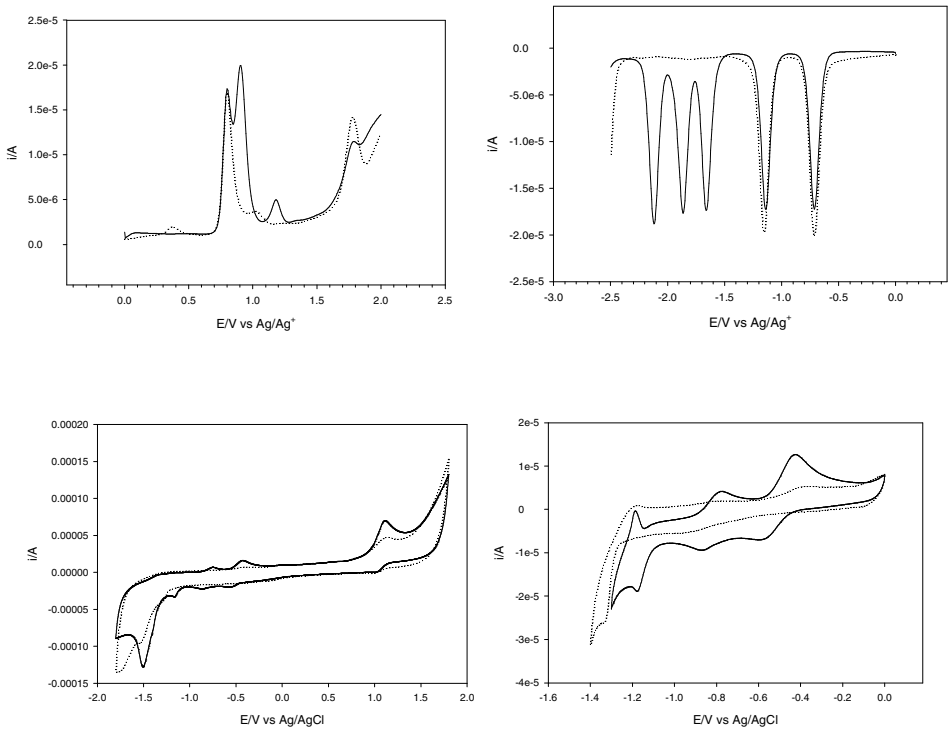


Figure S6. DPV curves (above, left: oxidation), DPV curves (above, right: reduction) of triad **1** (1×10^{-3} M) (solid line) and ligand **2** (1×10^{-3} M) (dashed line) in acetonitril, with Bu_4NPF_6 (0.1 M) as supporting electrolyte, glassy carbon disk as working electrode and Ag/AgCl as reference electrode. Cyclic voltammograms (v=0.1 V s^{-1}) of triad **1** (1×10^{-3} M) (bottom) in the absence (solid line) and in the presence (dashed line) of 1 equiv CB[8] in 0.1 M phosphate

buffered (PH 7.0) solution at room temperature, glassy carbon disk as working electrode, $Ag/AgNO_3$ as reference electrode, scan rate: v=0.1 V s^{-1}.

IV. UV-Vis of triad 1 with CB[8]

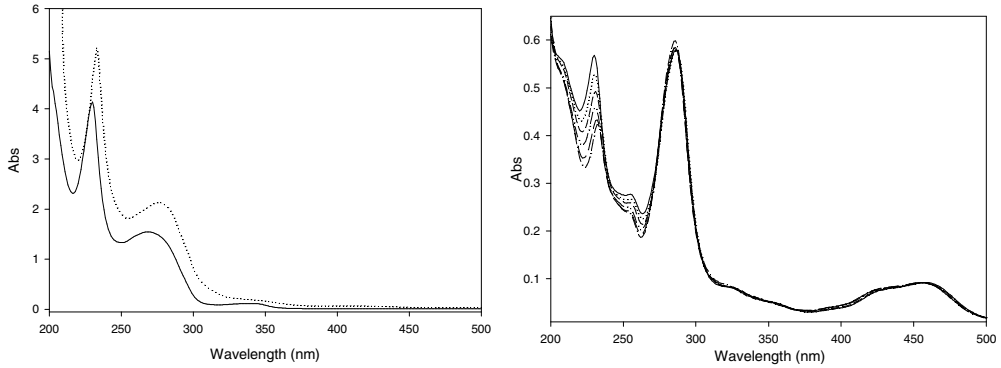


Figure S7. Absorption spectra of ligand **2** in the absence (left, solid line) and in the presence of 1.0 equiv (left, dashed line) of CB[8]. Absorption spectra of triad **1** in the absence (right, solid line) and in the presence of 0.2 equiv, 0.4 equiv, 0.6 equiv, 0.8 equiv, 1.0 equiv of CB[8] (right, dashed line) of CB[8].

Reference:

1. L. F. Cooley, S. L. Larson, C. M. Elliott, D. F. Kelley, *J. Phys. Chem.* **1991**, *95*, 10694-10700.
2. D. Zou, S. Andersson, R. Zhang, S. Sun, J. Pan, B. Åkermark, L. Sun, *Chem. Commun.* **2007**, 4734-4736.