

# **CHEMISTRY**

---

## **AN ASIAN JOURNAL**

### Supporting Information

© Copyright Wiley-VCH Verlag GmbH & Co. KGaA, 69451 Weinheim, 2012

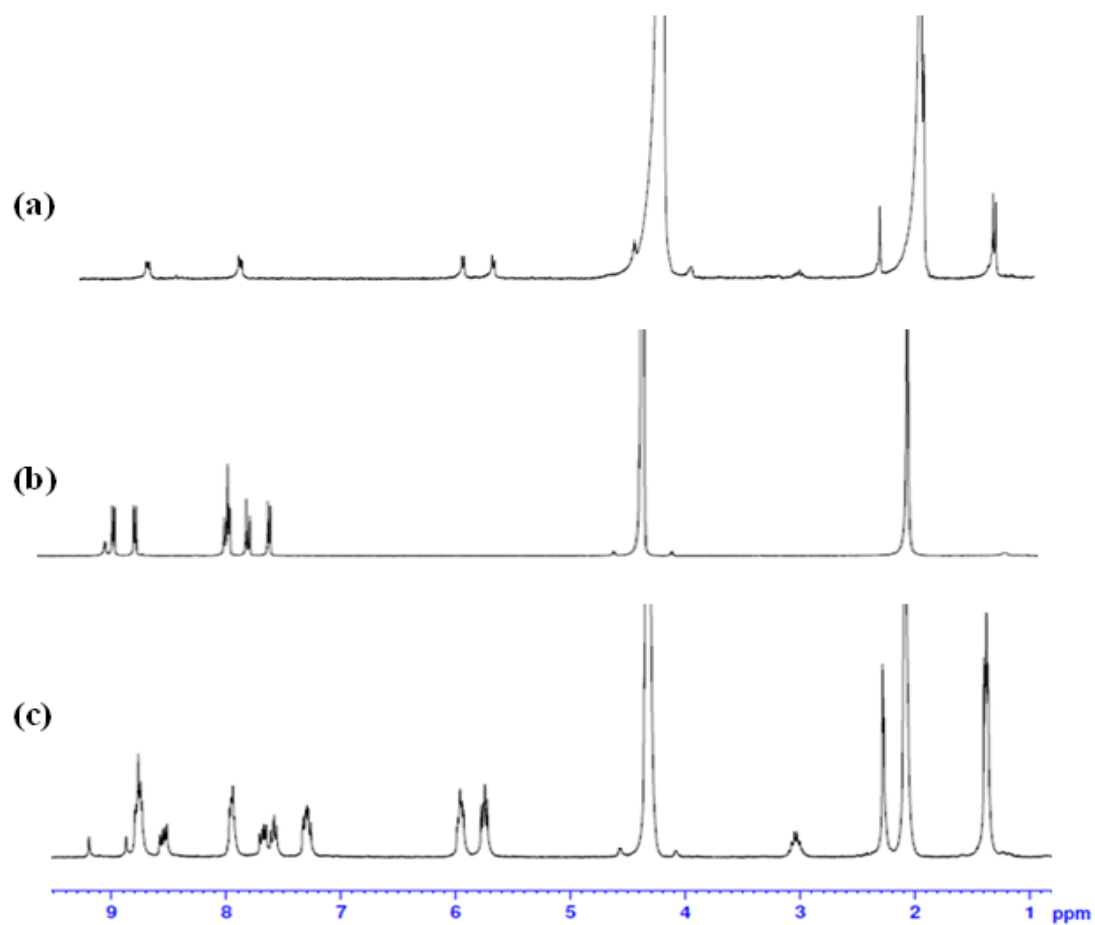
#### **Selective Detection of Multicarboxylate Anions based on “Turn on” Electron Transfer by Self-Assembled Molecular Rectangles**

**Anurag Mishra,<sup>[a]</sup> Sunmi Lee,<sup>[a]</sup> Hyunuk Kim,<sup>[b]</sup> Timothy R. Cook,<sup>[c]</sup> Peter J. Stang,<sup>[c]</sup> and Ki-Whan Chi\*<sup>[a]</sup>**

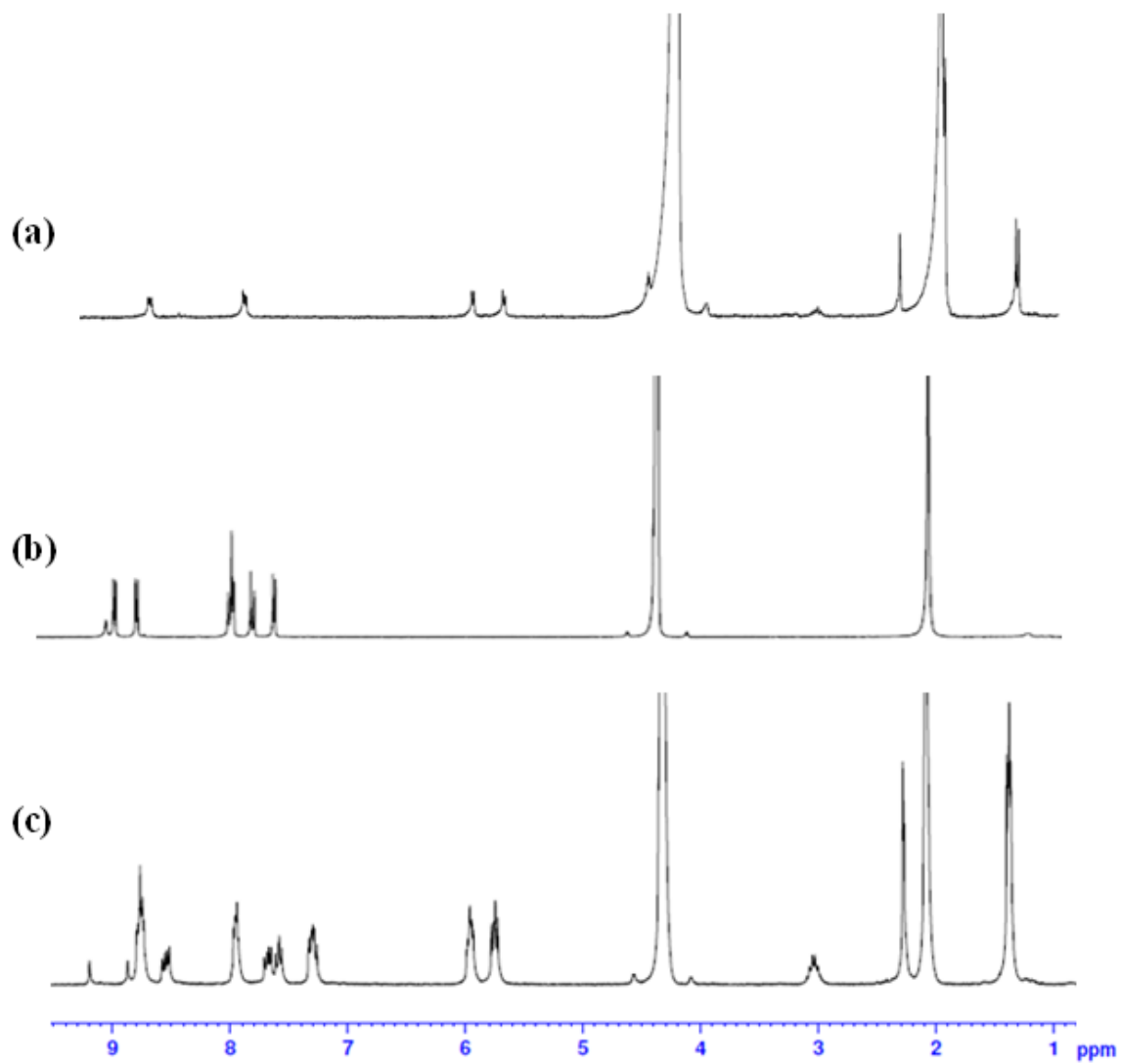
asia\_201200488\_sm\_miscellaneous\_information.pdf

## Table of Contents

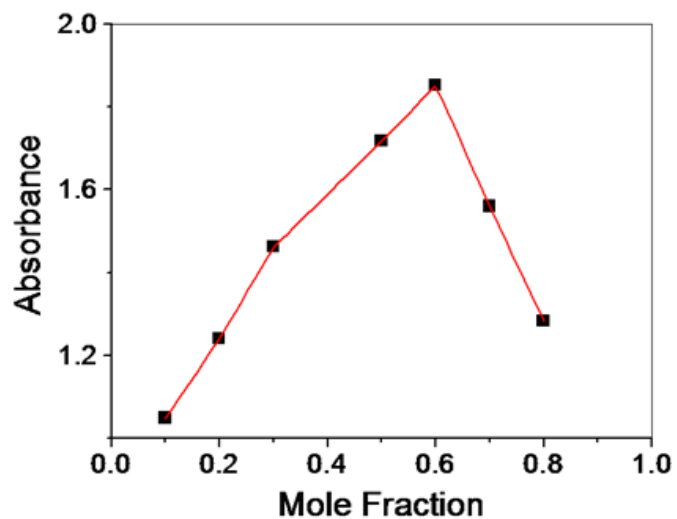
1. **Figure S1.** Comparison of the  $^1\text{H}$  NMR aromatic region of (a) Ru acceptor **2**, (b) amide ligand **1**, and (c) self-assembled [2+2] rectangle **4** in Nitromethane- $\text{d}_3$  solvent.
2. **Figure S2.** Comparison of the  $^1\text{H}$  NMR aromatic region of (a) Ru acceptor **3**, (b) amide ligand **1**, and (c) self-assembled [2+2] rectangle **5** in Nitromethane- $\text{d}_3$  solvent.
3. **Figure S3.** Job plot of tartrate anion titrations with **5**.
4. **Figure S4.**  $^1\text{H}$  NMR spectra of **5** in acetone with increasing amounts of  $[\text{Bu}_4\text{N}]_2$  oxalate. (a) 0, (b) 0.5, and (c) 1.0 equiv of  $[\text{Bu}_4\text{N}]_2$  oxalate.
5. **Table S1.** Crystal data and structure refinement for **5**.



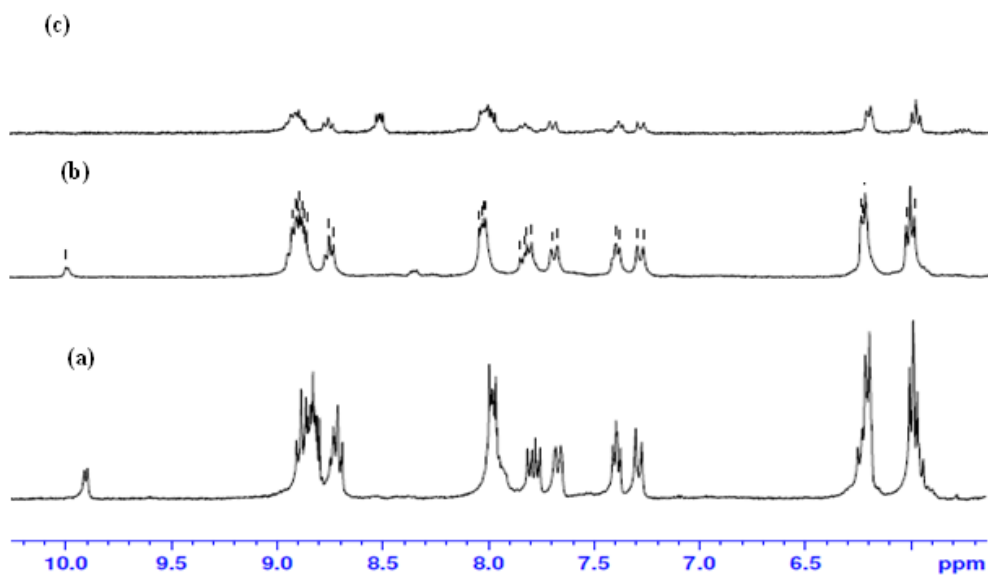
**Figure S1.** Comparison of the  $^1\text{H}$  NMR aromatic region of (a) Ru acceptor **2**, (b) amide ligand **1**, and (c) self-assembled [2+2] rectangle **4** in Nitromethane- $\text{d}_3$  solvent.



**Figure S2.** Comparison of the  $^1\text{H}$  NMR aromatic region of (a) Ru acceptor **3**, (b) amide ligand **1**, and (c) self-assembled [2+2] rectangle **5** in Nitromethane- $\text{d}_3$  solvent.



**Figure S3.** Job plot of tartrate anion titrations with **5**.



**Figure S4.**  $^1\text{H}$  NMR spectra of **5** in acetone with increasing amounts of  $[\text{Bu}_4\text{N}]_2$  oxalate. (a) 0, (b) 0.5, and (c) 1.0 equiv of  $[\text{Bu}_4\text{N}]_2$  oxalate.

**Table S1.** Crystal data and structure refinement for **5**.

Empirical formula	C130 H132 F12 N8 O30 Ru4 S4	
Formula weight	3046.96	
Temperature	100(2) K	
Wavelength	0.80000 Å	
Crystal system	Monoclinic	
Space group	<i>P21/c</i>	
Unit cell dimensions	$a = 18.232(4)$ Å	$\alpha = 90^\circ$
	$b = 20.125(4)$ Å	$\beta = 106.85(3)^\circ$
	$c = 18.433(4)$ Å	$\gamma = 90^\circ$
Volume	$6473(2)$ Å <sup>3</sup>	
Z	2	
Density (calculated)	1.563 g/cm <sup>3</sup>	
Absorption coefficient	0.838 mm <sup>-1</sup>	
F(000)	3112	
Crystal size	0.20 x 0.10 x 0.10 mm <sup>3</sup>	
Theta range for data collection	1.74 to 24.90°	
Index ranges	$-19 \leq h \leq 19$ , $-21 \leq k \leq 21$ , $-19 \leq l \leq 18$	
Reflections collected	28671	
Independent reflections	7714 [R(int) = 0.0325]	
Completeness to theta = 24.90°	97.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9209 and 0.8504	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	7714 / 154 / 853	
Goodness-of-fit on F <sup>2</sup>	1.686	
Final R indices [I > 2sigma(I)]	R1 = 0.1153, wR2 = 0.3480	
R indices (all data)	R1 = 0.1228, wR2 = 0.3574	
Extinction coefficient	0.016(2)	
Largest diff. peak and hole	1.654 and -0.814 e.Å <sup>-3</sup>	