Supporting Information

Coordination Driven Self-Assembly and Anticancer Activity of Molecular Rectangles Containing Octahedral Ruthenium Metal Centers

Vaishali Vajpayee,[†] Young Ho Song,[†] Yoon Jung Yang,[‡] Se Chan Kang,[‡] Hyunuk Kim,[±] In Su Kim,[†] Ming Wang,[ζ] Peter J. Stang,[*ζ] and Ki-Whan Chi[*†]*

[†] Department of Chemistry, University of Ulsan, Ulsan 680-749, Republic of Korea.

[‡] Department of Natural Medicine Resources, University of Semyung, Jecheon 390-711, Republic of Korea.

[±] Department of Chemistry, POSTECH, Pohang 690-784, Republic of Korea.

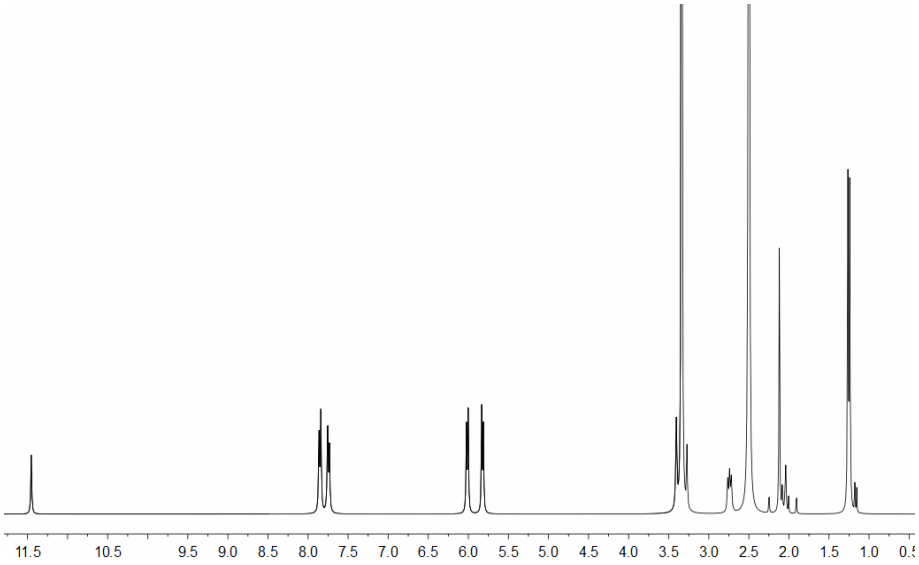
[ζ] Department of Chemistry, University of Utah, Salt Lake City, Utah 84112-0850, U.S.A.

[*]E-mail: kwchi@ulsan.ac.kr, sckang@semyung.ac.kr, stang@chem.utah.edu

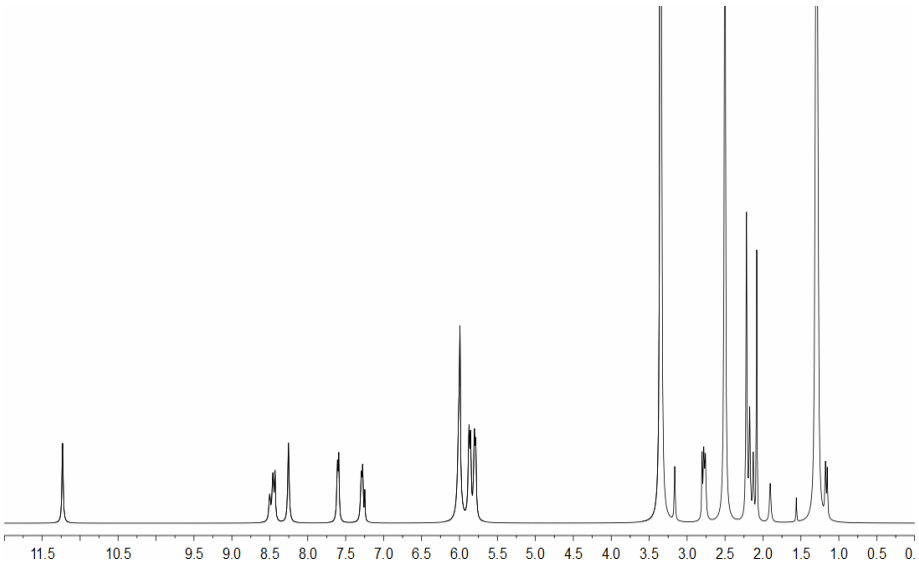
Table of Contents

Figure 1. ^{1}H NMR spectra of the metalla-rectangles **1** (a), **2** (b) and **3** (c).

(a)



(b)



(c)

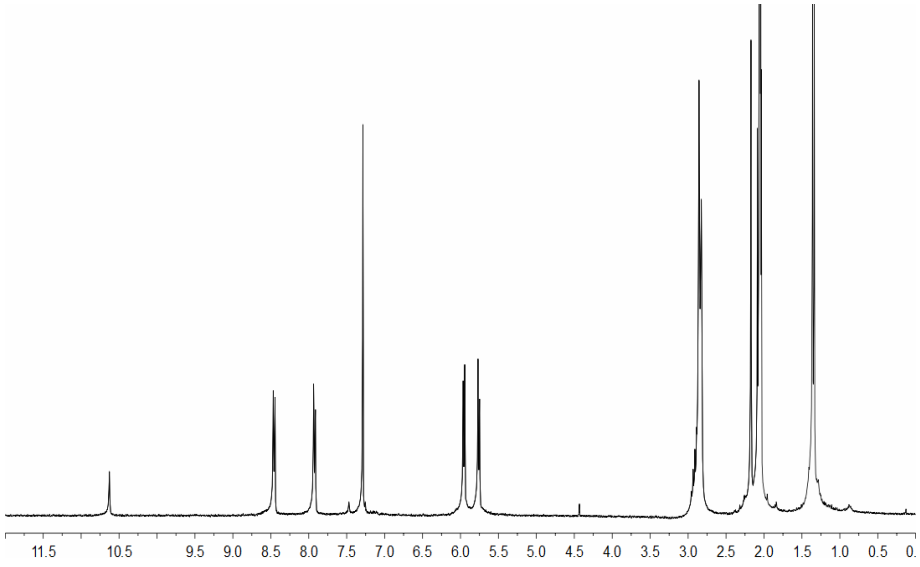
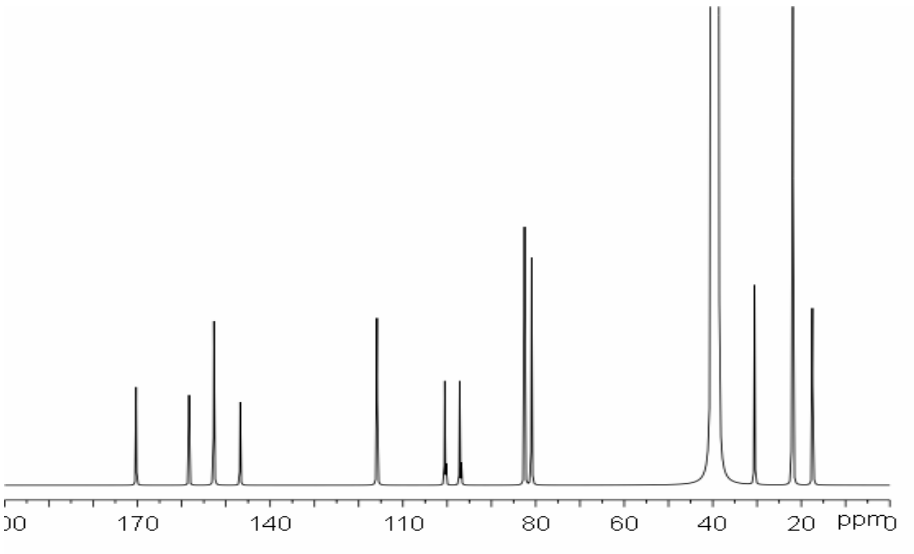
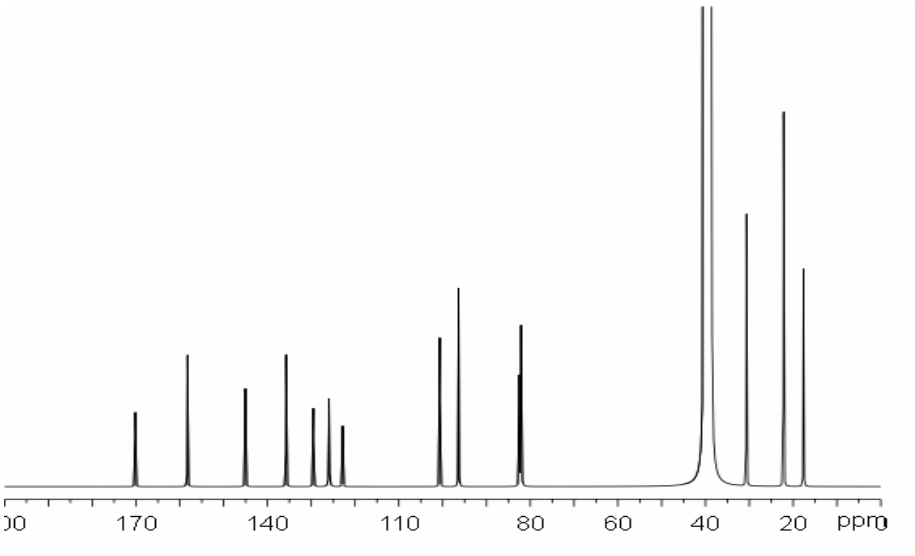


Figure 2. ^{13}C NMR spectra of the metalla-rectangles **1** (a), **2** (b) and **3** (c).

(a)



(b)



(c)

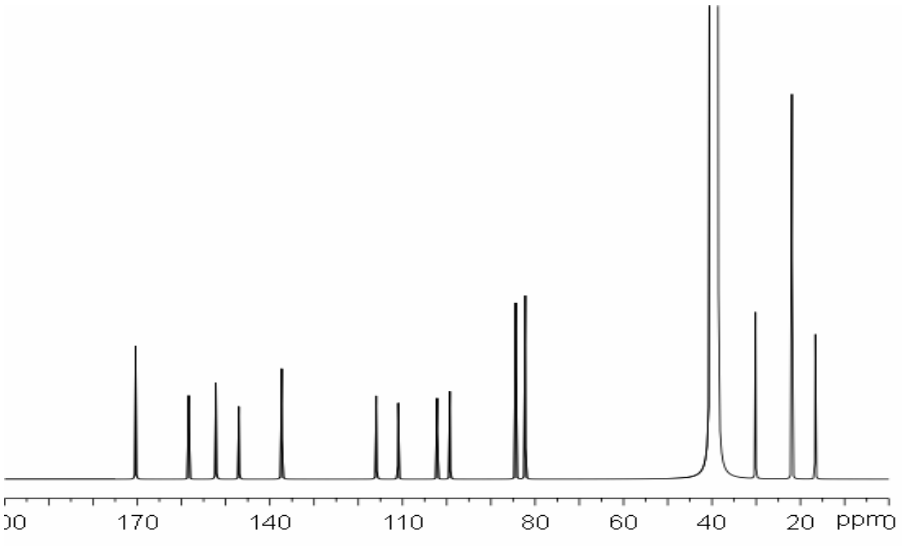
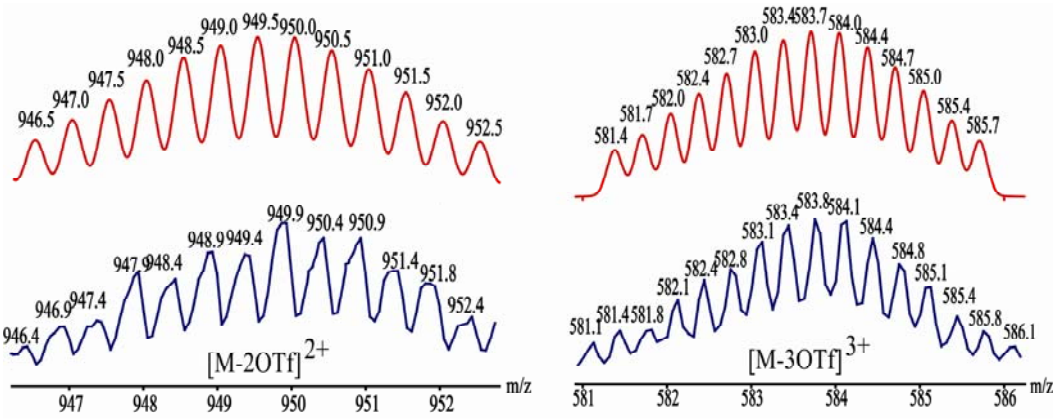
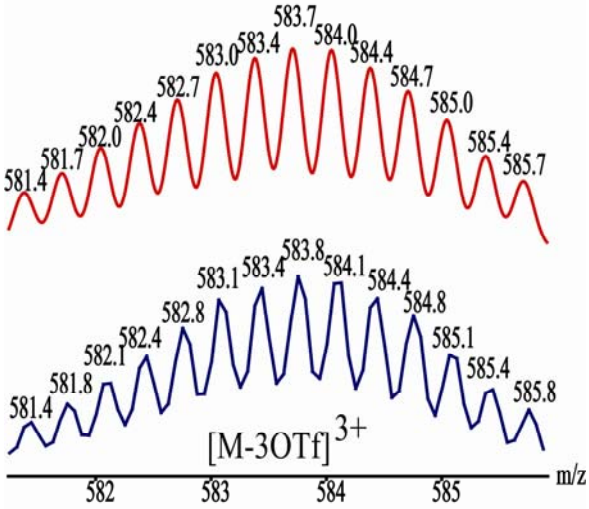


Figure 3. Calculated and experimental ESI-MS spectra of the metalla-rectangles **1**(a), **2** (b) and **3** (c).

(a)



(b)



(c)

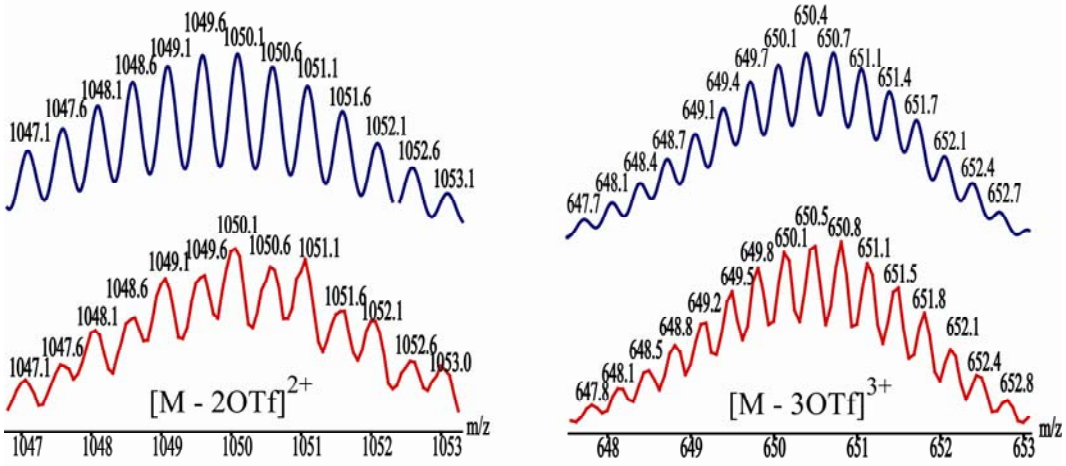


Table S1. Crystal data and structure refinement for **1** and **2.**

	1	**2**
Formula	$C_{76.12}$ $H_{86.80}$ F_{12} N_9 $O_{26.78}$ S_4 Ru_4	C_{73} H_{79} F_{12} N_9 O_{26} S_4 Ru_4
Fw	2316.79	2258.97
T, K	100(2) K	100(2)
λ, Å	0.900000	0.900000
Crystal syst	Monoclinic	Triclinic
Space group	$P2_1/n$	P-1
a, Å	13.827(3)	11.336(2)
b, Å	27.498(6)	17.650(4)
c, Å	24.766(5)	24.465(5)
α, deg	90	81.32(3)
β, deg	98.79(3)	83.65(3)
γ, deg	90	76.40(3)
Volume, $Å^3$	9306(3)	4688.9(16)
Z	4	2
Density, g/cm^3	1.654	1.600
μ, mm^{-1}	1.550	1.533
F(000)	4675	2272
Index ranges	$0\leq h\leq 15$, $-30\leq k\leq 30$, $-27\leq l\leq 27$	$-11\leq h\leq 11$, $-17\leq k\leq 17$, $-24\leq l\leq 24$
Independent reflections	12926 [R(int) = 0.0205]	8889 [R(int) = 0.0375]
GoF[a] on F^2	1.064	0.993
R_1,[b] wR_2[c] [I>2sigma(I)]	0.0631, 0.1880	0.0909, 0.2593
R_1, wR_2(all data)	0.0706, 0.1984	0.0994, 0.2681

[a]GoF = $\{\Sigma[w(F_o^2 - F_c^2)^2]/(n - p)\}^{1/2}$, where n and p denote the number of data points and the number of parameters, respectively. [b]$R_1 = (\Sigma||F_o|-|F_c||)/\Sigma|F_o|$. [c]$wR_2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$, where $w = 1/[\sigma^2(F_o^2) + (aP)^2 + (bP)]$ and $P = [\max(0, F_o^2) +2F_c^2]/3$.

Figure 4. Numbered crystal diagram for metalla-rectangle **1**(left) and **2**(right). Color codes: yellow = Ru, green = C, blue = N, red = O.

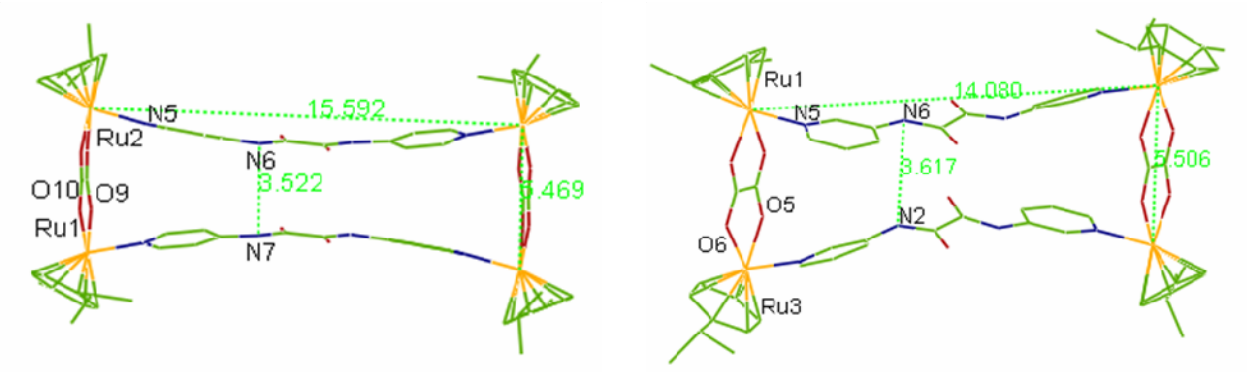


Table S2. Important Bond Lengths (Å) and Angles (º) for the metalla-rectangles **1** and **2**.

1

Ru(1)-O(9)	2.10(4)	Ru(2)-N(5)	2.11(5)
Ru(1)-O(10)	2.10(4)		
O(9)-Ru(1)-O(10)	78.7(16)	O(8)-Ru(1)-N(5)	84.1(18)

2

Ru(3)-O(5)	2.10(8)	Ru(1)-N(5)	2.10(9)
Ru(3)-O(6)	2.13(8)		
O(5)-Ru(3)-O(6)	79.0(3)	O(7)-Ru(1)-N(5)	83.2(3)

Table S3. Hydrogen bonds for **1** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2A)...O(3S)	0.88	2.04	2.872(7)	156.9
N(3)-H(3A)...O(2S)#2	0.88	2.25	3.083(7)	157.6
N(6)-H(6A)...O(7S)	0.88	2.19	3.032(7)	159.0
N(7)-H(7A)...O(9S)#1	0.88	2.11	2.905(7)	149.9

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z+2 #2 -x+2,-y,-z+2