Electronic Supporting Information (ESI)

A Family of Edge-Sharing Bioctahedral Diruthenium(III,III) Compounds Containing Ru-Ru Single Bond

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Table S1-1. Crystallographic data and structure refinement details for compounds **1**—**4.**

Compound	**1**	**2**	**3**	**4**
Empirical formula	$C_{16}H_{26}O_{10}Ru_2$	$C_{16}H_{20}F_6O_{10}Ru_2$	$C_{18}H_{18}F_{12}O_{10}Ru_2$	$C_{18}H_{30}O_{10}Ru_2$
Formula weight	580.51	688.45	824.45	608.52
Temperature (K)	200	150	150	180
Wavelength (Å)	1.34138	1.34138	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$
a [Å]	7.494(7)	7.9040(5)	8.6541(15)	7.8332(8)
b [Å]	17.150(15)	17.5442(11)	17.954(3)	17.5642(17)
c [Å]	7.979(5)	17.1910(10)	8.3730(14)	16.970(2)
β [°]	93.56(5)	110.411(3)	94.844(8)	90.706(5)
V [Å^3]	1023.5(14)	2234.2(2)	1296.3(4)	2334.6(4)
Z	2	4	2	4
ρ_{calcd} [g·cm^{-3}]	1.884	2.407	2.112	1.731
μ [mm^{-1}]	8.402	8.039	1.302	1.342
F(000)	580	1352	804	1224
GOF on F^2	1.027	1.053	1.074	0.999
Reflections collected	10077	25020	13798	24011
Reflections unique	1933	4232	2475	4440
$R_{(int)}$	0.0982	0.0677	0.1162	0.1471
R_1, wR_2 [$I>2\sigma(I)$][a]	0.0458, 0.0970	0.0368, 0.0926	0.0750, 0.1804	0.0590, 0.1409
R_1, wR_2[a] (all data)	0.0859, 0.1152	0.0535, 0.0985	0.1264, 0.2146	0.1070, 0.1643
$(\Delta\rho)_{max}$, $(\Delta\rho)_{min}$ [e/Å^3]	0.782, -1.035	0.816, -1.112	1.430，-2.284	1.277, -1.108

Table S1-2. Crystallographic data and structure refinement details for compounds **5**—**8.**

Compound	**5**	**6**	**7**	**8**
Empirical formula	$C_{18}H_{24}F_6O_{10}Ru_2$	$C_{20}H_{22}F_{12}O_{10}Ru_2$	$C_{18}H_{18}Cl_2F_6O_{10}Ru_2$	$C_{18}H_{16}Cl_2F_{12}O_{10}Ru_2$
Formula weight	716.51	852.50	757.34	893.34
Temperature (K)	150	200	293	180
Wavelength (Å)	1.34138	0.71073	1.34138	1.34138
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$
a [Å]	8.408(19)	8.7030(6)	9.314(15)	8.7048(4)
b [Å]	17.66(4)	18.5622(13)	17.92(3)	18.4734(8)
c [Å]	8.367(19)	8.6999(6)	8.011(15)	8.7051(4)
β [°]	99.14(10)	98.218(3)	108.34(5)	99.066(2)
V [Å^3]	1227(5)	1391.01(17)	1269(4)	1382.36
Z	2	2	2	2
ρ_{calcd} [g·cm^{-3}]	1.939	2.035	1.982	2.146
μ [mm^{-1}]	7.340	1.217	8.388	7.993
F(000)	708	836	740	868
GOF on F^2	1.068	1.077	1.083	1.046
Reflections collected	11804	32286	11642	17502
Reflections unique	2313	2627	2398	2613
$R_{(int)}$	0.1381	0.0964	0.1417	0.0459
R_1, wR_2 [$I>2\sigma(I)$][a]	0.0899, 0.2169	0.0423, 0.0925	0.0740, 0.1919	0.0272, 0.0693
R_1, wR_2 [a] (all data)	0.1153, 0.2306	0.0598, 0.1020	0.1567, 0.2295	0.0298, 0.0707
$(\Delta\rho)_{max}$, $(\Delta\rho)_{min}$ [e/Å^3]	1.692, -1.876	0.719, -1.285	1.212, -1.428	0.718, -0.813

Table S1-3. Crystallographic data and structure refinement details for compounds **9** and **10**

Compound	**9**	**10**
Empirical formula	$C_{26}H_{24}F_6O_{10}Ru_2$	$C_{14}H_{22}O_{10}Ru_2$
Formula weight	812.59	552.46
Temperature (K)	294	180
Wavelength (Å)	1.34138	1.34138
Crystal system	Triclinic	Monoclinic
Space group	$P\bar{1}$	$P2_1/c$
a [Å]	11.899(4)	9.6719(9)
b [Å]	14.482(4)	7.1673(5)
c [Å]	15.387(4)	14.9572(9)
α [°]	65.673(8)	90
β [°]	87.772(9)	119.200(5)
γ [°]	75.159(10)	90
V [Å^3]	2328.8(12)	905.09(13)
Z	3	2

ρ_{calcd} [g·cm^{-3}]	1.738	2.027
μ [mm^{-1}]	5.858	9.476
F(000)	1206	548
GOF on F^2	1.038	1.144
Reflections collected	29572	6507
Reflections unique	8756	1605
$R_{(int)}$	0.0435	0.0287
R_1, wR_2 [$I>2\sigma(I)$][a]	0.0478, 0.1336	0.0312, 0.0816
R_1, wR_2[a] (all data)	0.0525, 0.1366	0.0315, 0.0818
$(\Delta\rho)_{max}$, $(\Delta\rho)_{min}$ [e/Å^3]	1.260, -0.742	0.721, -0.712

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table S2-1. Selected bond distances (Å) and angles (˚) for compound **1**

Selected bond distances (Å)			
Ru(1)-Ru(1)#1	2.476(2)	O(3)-C(6)	1.284(9)
Ru(1)-O(5)	1.999(5)	O(4)-C(6)	1.271(9)
Ru(1)-O(1)	2.021(5)	O(5)-C(8)	1.434(8)
Ru(1)-O(2)	2.020(5)	C(1)-C(2)	1.376(10)
Ru(1)-O(3)	2.081(5)	C(1)-C(3)	1.403(10)
Ru(1)-O(4)#1	2.080(5)	C(2)-C(4)	1.516(10)
Ru(1)-O(5)#1	1.998(5)	C(3)-C(5)	1.493(10)
O(1)-C(2)	1.278(9)	C(6)-C(7)	1.499(10)
O(2)-C(3)	1.275(9)		
Selected angles (˚)			
O(5)-Ru(1)-O(5)#1	103.4(2)	O(3)-Ru(1)-Ru(1)#1	87.50(15)
O(5)-Ru(1)-O(1)	170.4(2)	O(4)#1-Ru(1)-Ru(1)#1	87.05(15)
O(5)#1-Ru(1)-O(1)	84.1(2)	C(2)-O(1)-Ru(1)	125.0(4)
O(5)-Ru(1)-O(2)	82.8(2)	C(3)-O(2)-Ru(1)	125.6(4)
O(5)#1-Ru(1)-O(2)	170.7(2)	C(6)-O(3)-Ru(1)	119.0(4)
O(1)-Ru(1)-O(2)	90.4(2)	C(6)-O(4)-Ru(1)#1	119.9(5)
O(5)-Ru(1)-O(3)	83.69(19)	C(8)-O(5)-Ru(1)	122.8(4)
O(5)#1-Ru(1)-O(3)	93.2(2)	C(8)-O(5)-Ru(1)#1	124.1(4)
O(1)-Ru(1)-O(3)	90.08(19)	Ru(1)-O(5)-Ru(1)#1	76.56(18)
O(2)-Ru(1)-O(3)	94.3(2)	C(2)-C(1)-C(3)	124.8(7)
O(5)-Ru(1)-O(4)#1	93.0(2)	O(1)-C(2)-C(1)	127.5(6)
O(5)#1-Ru(1)-O(4)#1	83.3(2)	O(1)-C(2)-C(4)	113.8(6)
O(1)-Ru(1)-O(4)#1	93.73(19)	C(1)-C(2)-C(4)	118.7(6)
O(2)-Ru(1)-O(4)#1	89.6(2)	O(2)-C(3)-C(1)	125.8(6)
O(3)-Ru(1)-O(4)#1	174.6(2)	O(2)-C(3)-C(5)	114.5(6)
O(5)-Ru(1)-Ru(1)#1	51.69(16)	C(1)-C(3)-C(5)	119.7(6)
O(5)#1-Ru(1)-Ru(1)#1	51.75(15)	O(4)-C(6)-O(3)	126.2(6)
O(1)-Ru(1)-Ru(1)#1	135.51(15)	O(4)-C(6)-C(7)	117.1(6)
O(2)-Ru(1)-Ru(1)#1	134.05(14)	O(3)-C(6)-C(7)	116.7(6)

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

Table S2-2. Selected bond distances (Å) and angles (˚) for compound **2**

Selected bond distances (Å)			
Ru(1)-Ru(2)	2.4663(5)	O(8)-C(10)	1.278(6)
Ru(1)-O(1)	1.987(3)	O(9)-C(13)	1.275(6)
Ru(1)-O(2)	1.991(3)	O(10)-C(15)	1.272(6)
Ru(1)-O(7)	2.023(3)	C(3)-C(4)	1.483(8)
Ru(1)-O(8)	2.024(3)	C(5)-C(6)	1.513(8)
Ru(1)-O(5)	2.072(3)	C(7)-C(8)	1.499(7)
Ru(1)-O(3)	2.079(3)	C(8)-C(9)	1.410(7)
Ru(2)-O(1)	1.988(3)	C(9)-C(10)	1.375(7)
Ru(2)-O(2)	1.986(3)	C(10)-C(11)	1.527(7)
Ru(2)-O(4)	2.058(3)	C(12)-C(13)	1.513(7)
Ru(2)-O(6)	2.062(3)	C(13)-C(14)	1.412(7)
Ru(2)-O(9)	2.014(3)	C(14)-C(15)	1.363(7)
Ru(2)-O(10)	2.031(3)	C(15)-C(16)	1.510(7)
O(1)-C(1)	1.446(6)	F(1)-C(11)	1.324(6)
O(2)-C(2)	1.440(6)	F(2)-C(11)	1.320(7)
O(3)-C(3)	1.272(6)	F(3)-C(11)	1.320(7)
O(4)-C(3)	1.289(6)	F(4)-C(16)	1.327(6)
O(5)-C(5)	1.269(6)	F(5)-C(16)	1.356(6)
O(6)-C(5)	1.274(6)	F(6)-C(16)	1.339(7)
O(7)-C(8)	1.281(6)		
Selected angles (˚)			
Ru(2)-Ru(1)-O(1)	51.67(9)	Ru(2)-O(1)-C2(1)	123.6(3)
Ru(2)-Ru(1)-O(2)	51.59(9)	Ru(1)-O(2)-Ru(2)	76.65(11)
Ru(2)-Ru(1)-O(3)	86.94(8)	Ru(1)-O(2)-C(2)	122.2(3)
Ru(2)-Ru(1)-O(5)	87.33(9)	Ru(2)-O(2)-C(2)	123.0(3)
Ru(2)-Ru(1)-O(7)	135.11(9)	Ru(1)-O(3)-C(3)	119.8(3)
Ru(2)-Ru(1)-O(8)	134.84(9)	Ru(2)-O(4)-C(3)	119.5(3)
O(1)-Ru(1)-O(2)	103.26(13)	Ru(1)-O(5)-C(5)	119.3(3)
O(1)-Ru(1)-O(3)	84.12(13)	Ru(2)-O(6)-C(5)	119.8(3)
O(1)-Ru(1)-O(5)	92.05(13)	Ru(1)-O(7)-C(8)	127.4(3)
O(1)-Ru(1)-O(7)	83.75(12)	Ru(1)-O(8)-C(10)	124.1(3)
O(1)-Ru(1)-O(8)	171.27(13)	Ru(2)-O(9)-C(13)	127.3(3)
O(2)-Ru(1)-O(3)	92.36(13)	Ru(2)-O(10)-C(15)	123.5(3)
O(2)-Ru(1)-O(5)	84.33(13)	O(3)-C(3)-O(4)	125.7(5)
O(2)-Ru(1)-O(7)	170.83(14)	O(3)-C(3)-C(4)	117.6(4)
O(2)-Ru(1)-O(8)	83.58(12)	O(4)-C(3)-C(4)	116.7(4)
O(3)-Ru(1)-O(5)	174.25(12)	O(5)-C(5)-O(6)	126.4(5)
O(3)-Ru(1)-O(7)	94.27(13)	O(5)-C(5)-C(6)	116.8(5)
O(3)-Ru(1)-O(8)	90.23(13)	O(6)-C(5)-C(6)	116.8(4)
O(5)-Ru(1)-O(7)	89.57(13)	O(7)-C(8)-C(7)	116.6(4)

O(5)-Ru(1)-O(8)	94.05(13)	O(7)-C(8)-C(9)	124.3(5)
O(7)-Ru(1)-O(8)	90.05(12)	C(7)-C(8)-C(9)	119.1(5)
Ru(1)-Ru(2)-O(1)	51.62(9)	C(8)-C(9)-C(10)	124.4(5)
Ru(1)-Ru(2)-O(2)	51.76(9)	O(8)-C(10)-C(9)	129.2(5)
Ru(1)-Ru(2)-O(4)	87.85(9)	O(8)-C(10)-C(11)	111.3(4)
Ru(1)-Ru(2)-O(6)	87.22(9)	C(9)-C(10)-C(11)	119.5(5)
Ru(1)-Ru(2)-O(9)	134.95(9)	F(1)-C(11)-F(2)	107.0(5)
Ru(1)-Ru(2)-O(10)	134.95(9)	F(1)-C(11)-F(3)	106.4(4)
O(1)-Ru(2)-O(2)	103.39(13)	F(1)-C(11)-C(10)	113.5(4)
O(1)-Ru(2)-O(4)	84.02(13)	F(2)-C(11)-F(3)	106.8(4)
O(1)-Ru(2)-O(6)	92.24(13)	F(2)-C(11)-C(10)	112.6(4)
O(1)-Ru(2)-O(9)	83.54(13)	F(3)-C(11)-C(10)	110.2(4)
O(1)-Ru(2)-O(10)	170.90(14)	O(9)-C(13)-C(12)	115.6(4)
O(2)-Ru(2)-O(4)	93.62(13)	O(9)-C(13)-C(14)	124.9(4)
O(2)-Ru(2)-O(6)	84.01(13)	C(12)-C(13)-C(14)	119.6(5)
O(2)-Ru(2)-O(9)	171.48(13)	C(13)-C(14)-C(15)	124.0(5)
O(2)-Ru(2)-O(10)	83.57(13)	O(10)-C(15)-C(14)	129.7(5)
O(4)-Ru(2)-O(6)	175.00(12)	O(10)-C(15)-C(16)	111.9(4)
O(4)-Ru(2)-O(9)	92.03(13)	C(14)-C(15)-C(16)	118.4(5)
O(4)-Ru(2)-O(10)	89.74(13)	F(4)-C(16)-F(5)	105.4(4)
O(6)-Ru(2)-O(9)	90.84(13)	F(4)-C(16)-C(6)	107.6(4)
O(6)-Ru(2)-O(10)	94.36(13)	F(4)-C(16)-C(15)	114.5(4)
O(9)-Ru(2)-O(10)	90.08(13)	F(5)-C(16)-F(6)	105.5(4)
Ru(1)-O(1)-Ru(2)	76.70(11)	F(5)-C(16)-C(15)	110.4(4)
Ru(1)-O(1)-C(1)	123.3(3)	F(6)-C(16)-C(15)	112.8(4)

Table S2-3. Selected bond distances (Å) and angles (°) for compound **3**

Selected bond distances (Å)			
Ru(1)-Ru(1)#1	2.4560(9)	O(5)-C(8)	1.258(10)
Ru(1)-O(3)	1.983(6)	C(1)-C(2)	1.492(15)
Ru(1)-O(4)	2.026(6)	C(3)-C(4)	1.455(16)
Ru(1)-O(5)	2.030(6)	C(5)-F(5)	1.290(11)
Ru(1)-O(1)	2.065(7)	C(5)-F(6)	1.290(12)
Ru(1)-O(2)	2.073(7)	C(5)-F(4)	1.298(13)
Ru(1)-O(3)#1	1.991(6)	C(5)-C(6)	1.540(13)
O(1)-C(1)#1	1.271(11)	C(6)-C(7)	1.370(14)
O(2)-C(1)	1.270(11)	C(7)-C(8)	1.390(13)
O(3)-C(3)	1.474(10)	C(8)-C(9)	1.513(14)
O(4)-C(6)	1.268(10)		
Selected angles (°)			
O(3)-Ru(1)-O(3)#1	103.7(2)	C(6)-O(4)-Ru(1)	76.4(2)
O(3)-Ru(1)-O(4)	171.9(3)	C(8)-O(5)-Ru(1)	125.8(6)
O(3)#1-Ru(1)-O(4)	83.3(2)	O(1)#1-C(1)-O(2)	126.3(6)
O(3)-Ru(1)-O(5)	84.4(2)	O(1)#1-C(1)-C(2)	126.2(9)

O(3)#1-Ru(1)-O(5)	171.0(2)	O(2)-C(1)-C(2)	116.7(9)
O(4)-Ru(1)-O(5)	88.9(2)	C(4)-C(3)-O(3)	117.1(8)
O(3)-Ru(1)-O(1)	84.2(2)	F(5)-C(5)-F(6)	110.3(9)
O(3)#1-Ru(1)-O(1)	92.1(3)	F(5)-C(5)-F(4)	107.8(9)
O(4)-Ru(1)-O(1)	91.5(3)	F(6)-C(5)-F(4)	107.9(9)
O(5)-Ru(1)-O(1)	92.8(3)	F(5)-C(5)-C(6)	104.8(10)
O(3)-Ru(1)-O(2)	92.1(2)	F(6)-C(5)-C(6)	112.9(9)
O(3)#1-Ru(1)-O(2)	85.1(2)	F(4)-C(5)-C(6)	112.4(8)
O(4)-Ru(1)-O(2)	92.7(2)	O(4)-C(6)-C(7)	110.6(8)
O(5)-Ru(1)-O(2)	90.7(3)	O(4)-C(6)-C(5)	128.0(9)
O(1)-Ru(1)-O(2)	174.7(2)	C(7)-C(6)-C(5)	110.8(8)
O(3)-Ru(1)-Ru(1)#1	51.97(17)	C(6)-C(7)-C(8)	121.1(8)
O(3)#1-Ru(1)-Ru(1)#1	51.69(16)	O(5)-C(8)-C(7)	123.3(9)
O(4)-Ru(1)-Ru(1)#1	134.84(18)	O(5)-C(8)-C(9)	127.5(9)
O(5)-Ru(1)-Ru(1)#1	136.23(16)	C(7)-C(8)-C(9)	111.9(8)
O(1)-Ru(1)-Ru(1)#1	86.99(16)	C(7)-C(8)-C(9)	120.7(9)
O(2)-Ru(1)-Ru(1)#1	87.72(15)	F(1)-C(9)-F(3)	106.7(9)
C(1)#1-O(1)-Ru(1)	120.1(6)	F(1)-C(9)-F(2)	106.9(9)
C(1)-O(2)-Ru(1)	118.9(6)	F(3)-C(9)-F(2)	106.2(9)
C(3)-O(3)-Ru(1)	123.9(5)	F(1)-C(9)-C(8)	112.5(9)
C(3)-O(3)-Ru(1)#1	122.3(5)	F(3)-C(9)-C(8)	111.3(8)
Ru(1)-O(3)-Ru(1)#1	76.4(2)	F(2)-C(9)-C(8)	112.8(9)

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

Table S2-4. Selected bond distances (Å) and angles (˚) for compound **4**

Selected bond distances (Å)			
Ru(1)-Ru(2)	2.4748(8)	O(6)-C(6)	1.270(10)
Ru(1)-O(1)	1.973(5)	O(7)-C(10)	1.279(10)
Ru(1)-O(2)	2.009(5)	O(8)-C(12)	1.274(10)
Ru(1)-O(8)	2.023(6)	O(9)-C(15)	1.320(10)
Ru(1)-O(7)	2.023(6)	O(10)-C(17)	1.303(9)
Ru(1)-O(3)	2.070(5)	C(3)-C(4)	1.508(12)
Ru(1)-O(5)	2.084(5)	C(4)-C(5)	1.502(15)
Ru(2)-O(1)	1.996(5)	C(6)-C(7)	1.491(13)
Ru(2)-O(2)	2.011(5)	C(7)-C(8)	1.488(15)
Ru(2)-O(4)	2.085(5)	C(9)-C(10)	1.499(14)
Ru(2)-O(6)	2.079(6)	C(10)-C(11)	1.406(14)
Ru(2)-O(9)	2.009(5)	C(11)-C(12)	1.394(14)
Ru(2)-O(10)	2.034(5)	C(12)-C(13)	1.512(14)
O(1)-C(1)	1.422(10)	C(14)-C(15)	1.479(12)
O(2)-C(2)	1.436(10)	C(15)-C(16)	1.388(12)
O(3)-C(3)	1.284(10)	C(16)-C(17)	1.356(13)
O(4)-C(3)	1.258(10)	C(17)-C(18)	1.514(12)
O(5)-C(6)	1.284(10)		

Selected angles (˚)			
Ru(2)-Ru(1)-O(1)	51.84(15)	O(6)-Ru(2)-O(9)	92.6(2)
Ru(2)-Ru(1)-O(2)	52.05(15)	O(6)-Ru(2)-O(10)	90.5(2)
Ru(2)-Ru(1)-O(3)	87.56(15)	O(9)-Ru(2)-O(10)	90.9(2)
Ru(2)-Ru(1)-O(5)	86.99(15)	Ru(1)-O(1)-Ru(2)	77.16(19)
Ru(2)-Ru(1)-O(7)	133.66(18)	Ru(1)-O(1)-C(1)	122.9(5)
Ru(2)-Ru(1)-O(8)	135.35(17)	Ru(2)-O(1)-C(1)	122.5(5)
O(1)-Ru(1)-O(2)	103.9(2)	Ru(1)-O(2)-Ru(2)	75.99(18)
O(1)-Ru(1)-O(3)	93.6(2)	Ru(1)-O(2)-C(2)	122.6(5)
O(1)-Ru(1)-O(5)	83.9(2)	Ru(2)-O(2)-C(2)	122.9(5)
O(1)-Ru(1)-O(7)	82.2(2)	Ru(1)-O(3)-C(3)	119.1(5)
O(1)-Ru(1)-O(8)	171.1(2)	Ru(2)-O(4)-C(3)	119.6(5)
O(2)-Ru(1)-O(3)	83.6(2)	Ru(1)-O(5)-C(6)	119.7(5)
O(2)-Ru(1)-O(5)	92.1(2)	Ru(2)-O(6)-C(6)	119.7(6)
O(2)-Ru(1)-O(7)	171.8(2)	Ru(1)-O(7)-C(10)	125.7(6)
O(2)-Ru(1)-O(8)	83.5(2)	Ru(1)-O(8)-C(12)	124.7(6)
O(3)-Ru(1)-O(5)	174.4(2)	Ru(2)-O(9)-C(15)	126.4(5)
O(3)-Ru(1)-O(7)	90.6(2)	Ru(2)-O(10)-(17)	125.0(5)
O(3)-Ru(1)-O(8)	92.1(2)	O(3)-C(3)-O(4)	126.7(8)
O(5)-Ru(1)-O(7)	94.1(2)	O(3)-C(3)-C(4)	115.8(7)
O(5)-Ru(1)-O(8)	90.9(2)	O(4)-C(3)-C(4)	117.5(7)
O(7)-Ru(1)-O(8)	91.0(2)	C(3)-C(4)-C(5)	110.7(8)
Ru(1)-Ru(2)-O(1)	51.01(15)	O(5)-C(6)-O(6)	126.0(8)
Ru(1)-Ru(2)-O(2)	51.96(15)	O(5)-C(6)-C(7)	116.0(8)
Ru(1)-Ru(2)-O(4)	86.82(15)	O(6)-C(6)-C(7)	118.0(8)
Ru(1)-Ru(2)-O(6)	87.51(15)	C(6)-C(7)-C(8)	113.4(8)
Ru(1)-Ru(2)-O(9)	134.03(15)	O(7)-C(10)-C(9)	115.7(9)
Ru(1)-Ru(2)-O(10)	135.04(16)	O(7)-C(10)-C(11)	125.1(9)
O(1)-Ru(2)-O(2)	103.0(2)	C(9)-C(10)-C(11)	119.1(8)
O(1)-Ru(2)-O(4)	92.3(2)	C(10)-C(11)-(12)	125.6(8)
O(1)-Ru(2)-O(6)	84.5(2)	O(8)-C(12)-C(11)	127.1(9)
O(1)-Ru(2)-O(9)	83.2(2)	O(8)-C(12)-(13)	114.4(8)
O(1)-Ru(2)-O(10)	172.1(2)	C(11)-C(12)-(13)	118.6(8)
O(2)-Ru(2)-O(4)	83.9(2)	O(9)-C(15)-C(14)	113.8(7)
O(2)-Ru(2)-O(6)	92.2(2)	O(9)-C(15)-C(16)	122.8(8)
O(2)-Ru(2)-O(9)	172.5(2)	C(14)-C(15)-C(16)	123.4(8)
O(2)-Ru(2)-O(10)	83.3(2)	C(15)-C(16)-C(17)	129.8(8)
O(4)-Ru(2)-O(6)	174.3(2)	O(10)-C(17)-C(16)	124.9(8)
O(4)-Ru(2)-O(9)	91.7(2)	O(10)-C(17)-C(18)	114.6(8)
O(4)-Ru(2)-O(10)	93.3(2)	C(16)-C(17)-C(18)	120.5(7)

Table S2-5. Selected bond distances (Å) and angles (˚) for compound **5**

Selected bond distances (Å)			
Ru(1)-Ru(1)#1	2.450(6)	O(5)-C(6)	1.254(17)

Ru(1)-O(1)	1.978(9)	F(1)-C(5)	1.361(17)
Ru(1)-O(3)	2.081(10)	F(2)-C(5)	1.293(17)
Ru(1)-O(4)	2.009(10)	F(3)-C(5)	1.314(17)
Ru(1)-O(5)	2.024(10)	C(2)-C(3)	1.50(2)
Ru(1)-O(1)#1	1.978(10)	C(3)-C(4)	1.50(2)
Ru(1)-O(2)#1	2.067(9)	C(5)-C(6)	1.531(18)
O(1)-C(1)	1.429(15)	C(6)-C(7)	1.39(2)
O(2)-C(2)	1.251(16)	C(7)-C(8)	1.384(19)
O(3)-C(2)	1.292(17)	C(8)-C(9)	1.51(2)
O(4)-C(8)	1.252(16)		
Selected angles (˚)			
O(1)-Ru(1)-O(1)#1	103.5(4)	Ru(1)-O(1)-Ru(1)#1	76.5(3)
O(1)-Ru(1)-O(4)	83.1(4)	C(2)-O(2)-Ru(1)#1	119.7(8)
O(1)#1-Ru(1)-O(4)	172.2(4)	C(2)-O(3)-Ru(1)	118.3(8)
O(1)-Ru(1)-O(5)	171.1(4)	C(8)-O(4)-Ru(1)	126.8(8)
O(1)#1-Ru(1)-O(5)	83.8(4)	C(6)-O(5)-Ru(1)	124.1(8)
O(4)-Ru(1)-O(5)	90.1(4)	O(2)-C(2)-O(3)	126.8(12)
O(1)-Ru(1)-O(2)#1	85.0(3)	O(2)-C(2)-C(3)	117.2(12)
O(1)#1-Ru(1)-O(2)#1	92.2(3)	O(3)-C(2)-C(3)	115.9(12)
O(4)-Ru(1)-O(2)#1	92.7(4)	C(2)-C(3)-C(4)	115.5(12)
O(5)-Ru(1)-O(2)#1	89.7(3)	F(2)-C(5)-F(3)	109.0(12)
O(1)-Ru(1)-O(3)	91.9(3)	F(2)-C(5)-F(1)	107.0(11)
O(1)#1-Ru(1)-O(3)	85.0(4)	F(3)-C(5)-F(1)	105.2(12)
O(4)-Ru(1)-O(3)	90.6(4)	F(2)-C(5)-C(6)	112.3(11)
O(5)-Ru(1)-O(3)	93.9(4)	F(3)-C(5)-C(6)	113.9(11)
O(2)#1-Ru(1)-O(3)	175.1(4)	F(1)-C(5)-C(6)	109.0(11)
O(1)-Ru(1)-Ru(1)#1	51.8(3)	O(5)-C(6)-C(7)	128.5(12)
O(1)#1-Ru(1)-Ru(1)#1	51.7(3)	O(5)-C(6)-C(5)	112.3(10)
O(4)-Ru(1)-Ru(1)#1	134.7(3)	C(7)-C(6)-C(5)	119.3(12)
O(5)-Ru(1)-Ru(1)#1	135.3(2)	C(8)-C(7)-C(6)	124.1(14)
O(2)#1-Ru(1)-Ru(1)#1	87.7(3)	O(4)-C(8)-C(7)	125.6(12)
O(3)-Ru(1)-Ru(1)#1	87.5(3)	O(4)-C(8)-C(9)	116.2(12)
C(1)-O(1)-Ru(1)	123.4(8)	C(7)-C(8)-C(9)	117.9(12)
C(1)-O(1)-Ru(1)#1	124.0(8)		

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

Table S2-6. Selected bond distances (Å) and angles (˚) for compound **6**

Selected bond distances (Å)			
Ru(1)-Ru(1)#1	2.4601(6)	C(2)-C(3)	1.517(11)
Ru(1)-O(3)	1.985(4)	C(4)-C(5)	1.492(10)
Ru(1)-O(5)	2.029(4)	C(6)-C(7)	1.391(10)
Ru(1)-O(4)	2.030(4)	C(6)-C(8)	1.396(10)
Ru(1)-O(1)	2.070(4)	C(7)-C(9)	1.527(9)
Ru(1)-O(2)#1	2.074(4)	C(8)-C(10)	1.521(10)

Ru(1)-O(3)#1	1.995(4)	C(9)-F(3)	1.314(9)
O(1)-C(1)	1.282(7)	C(9)-F(2)	1.308(8)
O(2)-C(1)	1.275(7)	C(9)-F(1)	1.315(9)
O(3)-C(4)	1.466(8)	C(10)-F(6)	1.310(10)
O(4)-C(7)	1.252(7)	C(10)-F(4)	1.247(9)
O(5)-C(8)	1.256(8)	C(10)-F(5)	1.254(11)
C(1)-C(2)	1.489(9)		
Selected #1ngles (˚)			
O(3)-Ru(1)-O(3)#1	103.64(16)	C(7)-O(4)-Ru(1)	126.3(4)
O(3)#1-Ru(1)-O(5)	170.85(16)	C(8)-O(5)-Ru(1)	126.3(4)
O(3)-Ru(1)-O(5)	84.48(16)	O(2)-C(1)-O(1)	125.5(5)
O(3)#1-Ru(1)-O(4)	83.47(16)	O(2)-C(1)-C(2)	117.8(5)
O(3)-Ru(1)-O(4)	171.94(17)	O(1)-C(1)-C(2)	116.7(5)
O(5)-Ru(1)-O(4)	88.74(16)	C(1)-C(2)-C(3)	114.1(6)
O(3)#1-Ru(1)-O(1)	85.36(17)	C(5)-C(4)-O(3)	109.5(5)
O(3)-Ru(1)-O(1)	91.94(17)	C(7)-C(6)-C(8)	121.8(6)
O(5)-Ru(1)-O(1)	90.22(17)	O(4)-C(7)-C(6)	128.5(6)
O(4)-Ru(1)-O(1)	92.44(16)	O(4)-C(7)-C(9)	112.8(6)
O(3)#1-Ru(1)-O(2)#1	92.12(17)	C(6)-C(7)-C(9)	118.7(6)
O(3)-Ru(1)-O(2)#1	84.16(17)	O(5)-C(8)-C(6)	128.2(6)
O(5)-Ru(1)-O(2)#1	92.91(17)	O(5)-C(8)-C(10)	113.4(6)
O(4)-Ru(1)-O(2)#1	91.86(16)	C(6)-C(8)-C(10)	118.4(6)
O(1)-Ru(1)-O(2)#1	174.74(15)	F(3)-C(9)-F(2)	106.7(6)
O(3)#1-Ru(1)-Ru(1)#1	51.65(11)	F(3)-C(9)-F(1)	106.7(6)
O(3)-Ru(1)-Ru(1)#1	51.99(12)	F(2)-C(9)-F(1)	106.7(7)
O(5)-Ru(1)-Ru(1)#1	136.29(11)	F(3)-C(9)-C(7)	113.8(6)
O(4)-Ru(1)-Ru(1)#1	134.98(12)	F(2)-C(9)-C(7)	112.0(6)
O(1)-Ru(1)-Ru(1)#1	87.81(11)	F(1)-C(9)-C(7)	110.6(6)
O(2)#1-Ru(1)-Ru(1)#1	87.01(11)	F(6)-C(10)-F(4)	103.2(8)
C(1)-O(1)-Ru(1)	119.4(4)	F(6)-C(10)-F(5)	102.3(7)
C(1)-O(2)-Ru(1)#1	120.2(4)	F(4)-C(10)-F(5)	111.2(9)
C(4)-O(3)-Ru(1)	123.0(4)	F(6)-C(10)-C(8)	110.5(7)
C(4)-O(3)-Ru(1)#1	122.1(4)	F(4)-C(10)-C(8)	115.3(7)
Ru(1)-O(3)-Ru(1)#1	76.36(15)	F(5)-C(10)-C(8)	110.5(7)

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

Table S2-7. Selected bond distances (Å) and angles (˚) for compound **7**

Selected bond distances (Å)			
Ru(1)-Ru(1)#1	2.495(5)	O(5)-C(5)	1.252(14)
Ru(1)-O(1)	1.997(8)	C(2)-C(3)	1.53(2)
Ru(1)-O(4)	2.040(9)	C(3)-Cl(1)	1.815(18)
Ru(1)-O(5)	2.053(8)	C(4)-C(5)	1.534(19)
Ru(1)-O(2)	2.082(9)	C(5)-C(6)	1.44(2)
Ru(1)-O(1)#1	2.021(9)	C(6)-C(7)	1.406(18)

Ru(1)-O(3)#1	2.099(10)	C(7)-C(8)	1.51(2)
O(1)-C(1)	1.474(18)	C(8)-F(3)	1.357(18)
O(2)-C(2)	1.307(15)	C(8)-F(1)	1.334(15)
O(3)-C(2)	1.264(15)	C(8)-F(2)	1.395(19)
O(4)-C(7)	1.292(13)		
Selected angles (˚)			
O(1)-Ru(1)-O(1)#1	103.3(3)	Ru(1)-O(1)-Ru(1)#1	76.8(3)
O(1)-Ru(1)-O(4)	83.7(3)	C(2)-O(2)-Ru(1)	119.5(8)
O(1)#1-Ru(1)-O(4)	171.6(3)	C(2)-O(3)-Ru(1)#1	119.4(8)
O(1)-Ru(1)-O(5)	170.8(3)	C(7)-O(4)-Ru(1)	125.8(8)
O(1)#1-Ru(1)-O(5)	84.2(3)	C(5)-O(5)-Ru(1)	128.4(8)
O(4)-Ru(1)-O(5)	89.4(3)	O(3)-C(2)-O(2)	126.5(12)
O(1)-Ru(1)-O(2)	83.6(3)	O(3)-C(2)-C(3)	114.9(12)
O(1)#1-Ru(1)-O(2)	92.8(3)	O(2)-C(2)-C(3)	118.6(12)
O(4)-Ru(1)-O(2)	92.8(4)	C(2)-C(3)-Cl(1)	110.7(11)
O(5)-Ru(1)-O(2)	90.8(3)	O(5)-C(5)-C(6)	124.1(11)
O(1)-Ru(1)-O(3)#1	92.5(3)	O(5)-C(5)-C(4)	115.6(12)
O(1)#1-Ru(1)-O(3)#1	84.3(3)	C(6)-C(5)-C(4)	120.3(10)
O(4)-Ru(1)-O(3)#1	90.7(4)	C(7)-C(6)-C(5)	125.0(10)
O(5)-Ru(1)-O(3)#1	93.6(3)	O(4)-C(7)-C(6)	126.7(12)
O(2)-Ru(1)-O(3)#1	174.5(3)	O(4)-C(7)-C(8)	114.5(10)
O(1)-Ru(1)-Ru(1)#1	52.1(2)	C(6)-C(7)-C(8)	118.9(10)
O(1)#1-Ru(1)-Ru(1)#1	51.2(2)	F(3)-C(8)-F(1)	108.1(12)
O(4)-Ru(1)-Ru(1)#1	135.5(2)	F(3)-C(8)-F(2)	102.5(12)
O(5)-Ru(1)-Ru(1)#1	135.1(2)	F(1)-C(8)-F(2)	106.3(12)
O(2)-Ru(1)-Ru(1)#1	87.1(2)	F(3)-C(8)-C(7)	112.9(11)
O(3)#1-Ru(1)-Ru(1)#1	87.4(2)	F(1)-C(8)-C(7)	117.1(12)
C(1)-O(1)-Ru(1)	122.7(7)	F(2)-C(8)-C(7)	108.8(11)
C(1)-O(1)-Ru(1)#1	121.7(7)		

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

Table S2-8. Selected bond distances (Å) and angles (˚) for compound **8**

Selected bond distances (Å)			
Ru(1)-Ru(1)#1	2.4617(5)	C(1)-C(2)	1.494(7)
Ru(1)-O(1)	1.988(3)	C(3)-C(4)	1.507(6)
Ru(1)-O(1)#1	1.986(3)	C(5)-F(1)	1.305(6)
Ru(1)-O(2)	2.068(3)	C(5)-F(3)	1.311(5)
Ru(1)-O(4)	2.021(3)	C(5)-F(2)	1.317(6)
Ru(1)-O(5)	2.025(3)	C(5)-C(6)	1.530(6)
Ru(1)-O(3)#1	2.067(3)	C(6)-C(7)	1.387(6)
O(1)-C(1)	1.465(5)	C(7)-C(8)	1.398(6)
O(2)-C(3)	1.273(4)	C(8)-C(9)	1.526(6)
O(3)-C(3)	1.271(4)	C(9)-F(5)	1.265(6)
O(4)-C(6)	1.259(5)	C(9)-F(4)	1.270(5)

O(5)-C(8)	1.262(5)	C(9)-F(6)	1.297(6)
Cl(1)-C(4)	1.750(5)		
Selected angles (˚)			
O(1)#1-Ru(1)-O(1)	103.44(10)	C(6)-O(4)-Ru(1)	126.7(3)
O(1)#1-Ru(1)-O(4)	83.44(10)	C(8)-O(5)-Ru(1)	126.2(3)
O(1)-Ru(1)-O(4)	172.16(11)	O(1)-C(1)-C(2)	109.2(3)
O(1)#1-Ru(1)-O(5)	171.09(10)	O(3)-C(3)-O(2)	126.9(3)
O(1)-Ru(1)-O(5)	84.62(10)	O(3)-C(3)-C(4)	117.9(3)
O(4)-Ru(1)-O(5)	88.78(11)	O(2)-C(3)-C(4)	115.1(3)
O(1)#1-Ru(1)-O(3)#1	92.18(10)	C(3)-C(4)-Cl(1)	112.4(3)
O(1)-Ru(1)-O(3)#1	84.22(10)	F(1)-C(5)-F(3)	107.0(4)
O(4)-Ru(1)-O(3)#1	91.84(10)	F(1)-C(5)-F(2)	106.4(4)
O(5)-Ru(1)-O(3)#1	92.41(10)	F(3)-C(5)-F(2)	107.5(3)
O(1)#1-Ru(1)-O(2)	85.47(10)	F(1)-C(5)-C(6)	112.1(3)
O(1)-Ru(1)-O(2)	91.76(10)	F(3)-C(5)-C(6)	113.3(4)
O(4)-Ru(1)-O(2)	92.55(10)	F(2)-C(5)-C(6)	110.1(4)
O(5)-Ru(1)-O(2)	90.56(10)	O(4)-C(6)-C(7)	128.4(4)
O(3)#1-Ru(1)-O(2)	174.75(10)	O(4)-C(6)-C(5)	112.7(3)
O(1)#1-Ru(1)-Ru(1)#1	51.76(7)	C(7)-C(6)-C(5)	118.9(3)
O(1)-Ru(1)-Ru(1)#1	51.69(7)	C(6)-C(7)-C(8)	121.4(4)
O(4)-Ru(1)-Ru(1)#1	135.06(8)	O(5)-C(8)-C(7)	128.5(4)
O(5)-Ru(1)-Ru(1)#1	136.16(8)	O(5)-C(8)-C(9)	113.0(4)
O(3)#1-Ru(1)-Ru(1)#1	87.09(7)	C(7)-C(8)-C(9)	118.5(3)
O(2)-Ru(1)-Ru(1)#1	87.77(7)	F(5)-C(9)-F(4)	110.5(5)
C(1)-O(1)-Ru(1)#1	122.5(2)	F(5)-C(9)-F(6)	104.0(5)
C(1)-O(1)-Ru(1)	122.7(2)	F(4)-C(9)-F(6)	104.0(5)
Ru(1)#1-O(1)-Ru(1)	76.56(9)	F(5)-C(9)-C(8)	112.5(4)
C(3)-O(2)-Ru(1)	118.6(2)	F(4)-C(9)-C(8)	114.0(4)
C(3)-O(3)-Ru(1)#1	119.5(2)	F(6)-C(9)-C(8)	110.9(4)

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

Table S2-9. Selected bond distances (Å) and angles (˚) for compound **9**

Selected bond distances (Å)			
Ru(1)-Ru(1)#1	2.4650(10)	C(3)-C(8)	1.364(11)
Ru(2)-Ru(3)	2.4668(10)	C(3)-C(4)	1.382(9)
Ru(1)-O(1)	1.992(4)	C(4)-C(5)	1.390(12)
Ru(1)-O(1)#1	1.991(4)	C(5)-C(6)	1.348(13)
Ru(1)-O(5)	2.019(4)	C(6)-C(7)	1.364(19)
Ru(1)-O(4)	2.030(4)	C(7)-C(8)	1.375(17)
Ru(1)-O(2)	2.065(4)	C(9)-C(10)	1.548(13)
Ru(1)-O(3)#1	2.079(4)	C(10)-C(11)	1.389(11)
Ru(2)-O(6)	1.988(4)	C(11)-C(12)	1.357(13)
Ru(3)-O(6)	2.000(4)	C(12)-C(13)	1.504(12)
Ru(2)-O(12)	2.026(4)	C(13)-F(1)	1.20(12)

Ru(2)-O(13)	2.026(4)	C(13)-F(2)	1.30(12)
Ru(3)-O(9)	2.069(5)	C(13)-F(3)	1.338(18)
Ru(2)-O(8)	2.068(5)	C(17)-C(18)	1.381(12)
O(1)-C(1)	1.443(8)	C(17)-C(22)	1.394(11)
O(2)-C(2)	1.274(7)	C(18)-C(19)	1.377(17)
O(3)-C(2)	1.273(7)	C(19)-C(20)	1.36(2)
O(4)-C(12)	1.253(9)	C(20)-C(21)	1.35(2)
O(5)-C(10)	1.262(8)	C(21)-C(22)	1.407(14)
C(2)-C(3)	1.491(9)	C(30)-C(31)	1.534(11)
O6-C14	1.432(7)	C(31)-C(32)	1.383(10)
O8-C16	1.287(9)	C(32)-C(33)	1.375(10)
O9-C16	1.276(9)	C(33)-C(34)	1.491(12)
O12-C31	1.248(7)	F(4)-C(34)	1.319(13)
O13-C33	1.276(8)	F(5)-C(34)	1.320(16)
C16-C17	1.481(10)	F6-C(34)	1.240(19)
Selected angles (˚)			
O(1)-Ru(1)-O(1)#1	103.53(17)	C(12)-O(4)-Ru(1)	123.9(5)
O(1)-Ru(1)-O(5)	171.30(17)	C(10)-O(5)-Ru(1)	125.8(4)
O(1)#1-Ru(1)-O(5)	83.59(17)	O(2)-C(2)-O(3)	126.7(6)
O(1)-Ru(1)-O(4)	83.76(18)	O(2)-C(2)-C(3)	116.8(5)
O(1)#1-Ru(1)-O(4)	171.97(18)	O(3)-C(2)-C(3)	116.5(5)
O(5)-Ru(1)-O(4)	89.45(18)	C(8)-C(3)-C(4)	118.3(7)
O(1)-Ru(1)-O(2)	83.89(17)	C(8)-C(3)-C(2)	120.3(6)
O(1)#1-Ru(1)-O(2)	93.43(17)	C(4)-C(3)-C(2)	121.4(6)
O(5)-Ru(1)-O(2)	90.77(17)	C(3)-C(4)-C(5)	121.3(7)
O(4)-Ru(1)-O(2)	90.67(18)	C(6)-C(5)-C(4)	119.3(9)
O(1)-Ru(1)-O(3)#1	92.96(17)	C(5)-C(6)-C(7)	119.7(10)
O(1)#1-Ru(1)-O(3)#1	83.20(17)	C(8)-C(7)-C(6)	121.5(11)
O(5)-Ru(1)-O(3)#1	92.84(17)	C(3)-C(8)-C(7)	119.9(10)
O(4)-Ru(1)-O(3)#1	93.18(18)	O(5)-C(10)-C(11)	126.2(7)
O(2)-Ru(1)-O(3)#1	174.75(16)	O(5)-C(10)-C(9)	112.9(7)
O(1)-Ru(1)-Ru(1)#1	51.76(12)	C(11)-C(10)-C(9)	120.9(8)
O(1)#1-Ru(1)-Ru(1)#1	51.77(12)	C(12)-C(11)-C(10)	124.2(8)
O(5)-Ru(1)-Ru(1)#1	135.11(12)	O(4)-C(12)-C(11)	129.1(7)
O(4)-Ru(1)-Ru(1)#1	135.41(14)	O(4)-C(12)-C(13)	112.3(9)
O(2)-Ru(1)-Ru(1)#1	87.85(12)	C(11)-C(12)-C(13)	118.7(9)
O(3)#1-Ru(1)-Ru(1)#1	86.91(12)	F(1)-C(13)-F(2)	111.7(12)
C(1)-O(1)-Ru(1)	120.6(4)	F(1)-C(13)-F(3)	103.7(13)
C(1)-O(1)-Ru(1)#1	122.3(4)	F(2)-C(13)-F(3)	100.2(12)
Ru(1)-O(1)-Ru(1)#1	76.47(15)	F(1)-C(13)-C(12)	115.7(12)
C(2)-O(2)-Ru(1)	119.1(4)	F(2)-C(13)-C(12)	114.0(12)
C(2)-O(3)-Ru(1)#1	119.4(4)	F(3)-C(13)-C(12)	109.8(9)
O(6)-Ru(2)-O(7)	103.65(15)	C(31)-O(12)-Ru(2)	126.6(4)
O(6)-Ru(2)-O(12)	83.77(16)	C(33)-O(13)-Ru(2)	123.3(4)

O(7)-Ru(2)-O(12)	170.86(16)	O(9)-C(16)-O(8)	125.0(5)
O(6)-Ru(2)-O(13)	170.34(16)	O(9)-C(16)-C(17)	118.2(5)
O(7)-Ru(2)-O(13)	83.96(17)	O(8)-C(16)-C(17)	116.8(6)
O(12)-Ru(2)-O(13)	89.26(17)	C(18)-C(17)-C(22)	119.4(7)
O(6)-Ru(2)-O(8)	83.74(16)	C(18)-C(17)-C(16)	122.2(7)
O(7)-Ru(2)-O(8)	93.44(17)	C(22)-C(17)-C(16)	118.3(7)
O(12)-Ru(2)-O(8)	92.67(16)	C(19)-C(18)-C(17)	119.4(9)
O(13)-Ru(2)-O(8)	89.93(17)	C(20)-C(19)-C(18)	121.5(10)
O(6)-Ru(2)-O(10)	91.89(15)	C(21)-C(20)-C(19)	120.4(9)
O(7)-Ru(2)-O(10)	83.89(16)	C(20)-C(21)-C(22)	119.7(10)
O(12)-Ru(2)-O(10)	90.61(15)	C(17)-C(22)-C(21)	119.7(9)
O(13)-Ru(2)-O(10)	94.88(16)	O(13)-C(33)-C(32)	128.4(6)
O(8)-Ru(2)-O(10)	174.22(15)	O(13)-C(33)-C(34)	111.4(7)
O(6)-Ru(2)-Ru(3)	52.01(11)	C(33)-C(32)-C(31)	123.7(6)
O(7)-Ru(2)-Ru(3)	51.64(11)	C(32)-C(33)-C(34)	120.1(7)
O(12)-Ru(2)-Ru(3)	135.52(12)	O(12)-C(31)-C(32)	126.3(6)
O(13)-Ru(2)-Ru(3)	135.21(12)	O(12)-C(31)-C(30)	114.3(6)
O(8)-Ru(2)-Ru(3)	87.51(11)	C(32)-C(31)-C(30)	119.4(6)
O(9)-Ru(3)-Ru(2)	87.08(11)	F(6)-C(34)-F(5)	103.8(12)
C(14)-O(6)-Ru(2)	122.9(3)	F(6)-C(34)-F(4)	110.0(9)
C(14)-O(6)-Ru(3)	121.7(4)	F(5)-C(34)-F(4)	98.4(9)
Ru(2)-O(6)-Ru(3)	76.44(13)	F(6)-C(34)-C(33)	116.5(8)
C(16)-O(8)-Ru(2)	119.5(4)	F(5)-C(34)-C(33)	111.1(8)
C(16)-O(9)-Ru(3)	120.3(4)	F(4)-C(34)-C(33)	115.0(9)

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

Table S2-10. Selected bond distances (Å) and angles (˚) for compound **10**

Selected bond distances (Å)			
Ru(1)-Ru(1)#1	2.4771(4)	O(2)-C(2)	1.261(4)
Ru(1)-O(1)	2.003(2)	O(3)-C(2)	1.264(5)
Ru(1)-O(1)#1	1.999(2)	O(4)-C(4)	1.280(4)
Ru(1)-O(2)	2.086(2)	O(5)-C(6)	1.282(4)
Ru(1)-O(4)	2.022(3)	C(3)-C(4)	1.496(4)
Ru(1)-O(5)	2.013(2)	C(4)-C(5)	1.399(4)
Ru(1)-O(3)#1	2.077(2)	C(5)-C(6)	1.386(4)
O(1)-C(1)	1.429(4)	C(6)-C(7)	1.494(4)
Selected angles (˚)			
O(1)#1-Ru(1)-O(1)	103.51(9)	O(4)-Ru(1)-Ru(1)#1	135.60(8)
O(1)#1-Ru(1)-O(5)	82.71(9)	O(3)#1-Ru(1)-Ru(1)#1	87.49(6)
O(1)-Ru(1)-O(5)	172.43(9)	O(2)-Ru(1)-Ru(1)#1	86.87(6)
O(1)#1-Ru(1)-O(4)	171.38(9)	C(1)-O(1)-Ru(1)#1	121.8(2)
O(1)-Ru(1)-O(4)	84.08(10)	C(1)-O(1)-Ru(1)	122.9(2)
O(5)-Ru(1)-O(4)	90.06(10)	Ru(1)#1-O(1)-Ru(1)	76.49(8)
O(1)#1-Ru(1)-O(3)#1	83.49(9)	C(2)-O(2)-Ru(1)	118.6(2)

O(1)-Ru(1)-O(3)#1	93.38(9)	C(2)-O(3)-Ru(1)#1	118.4(2)
O(5)-Ru(1)-O(3)#1	91.60(9)	C(4)-O(4)-Ru(1)	125.83(19)
O(4)-Ru(1)-O(3)#1	92.07(9)	C(6)-O(5)-Ru(1)	125.57(18)
O(1)#1-Ru(1)-O(2)	92.87(9)	O(2)-C(2)-O(3)	128.3(3)
O(1)-Ru(1)-O(2)	83.25(9)	O(4)-C(4)-C(5)	125.0(3)
O(5)-Ru(1)-O(2)	92.22(9)	O(4)-C(4)-C(3)	115.3(3)
O(4)-Ru(1)-O(2)	92.07(9)	C(5)-C(4)-C(3)	119.7(3)
O(3)#1-Ru(1)-O(2)	174.36(9)	C(6)-C(5)-C(4)	126.1(3)
O(1)#1-Ru(1)-Ru(1)#1	51.83(6)	O(5)-C(6)-C(5)	125.5(3)
O(1)-Ru(1)-Ru(1)#1	51.69(6)	O(5)-C(6)-C(7)	114.4(2)
O(5)-Ru(1)-Ru(1)#1	134.35(6)	C(5)-C(6)-C(7)	120.1(3)

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

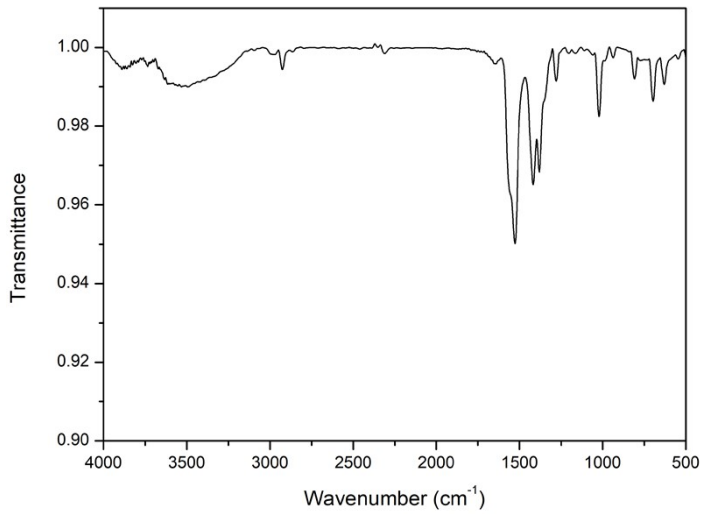

Fig. S1-1 IR spectra of compound **1**.

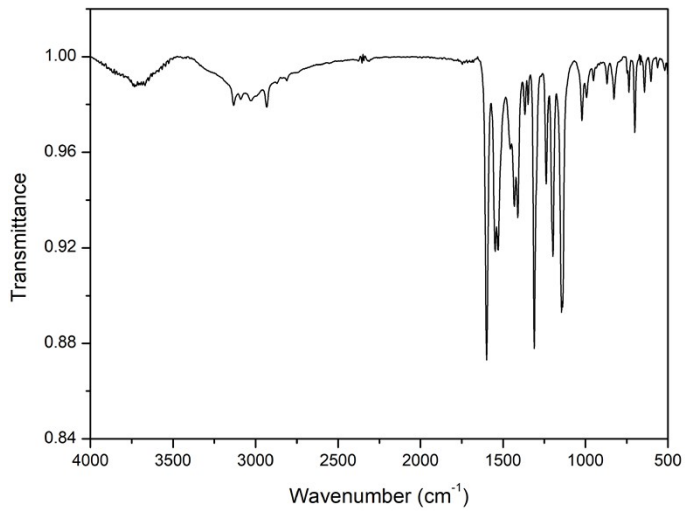

Fig S1-2. IR spectra of compound **2**.

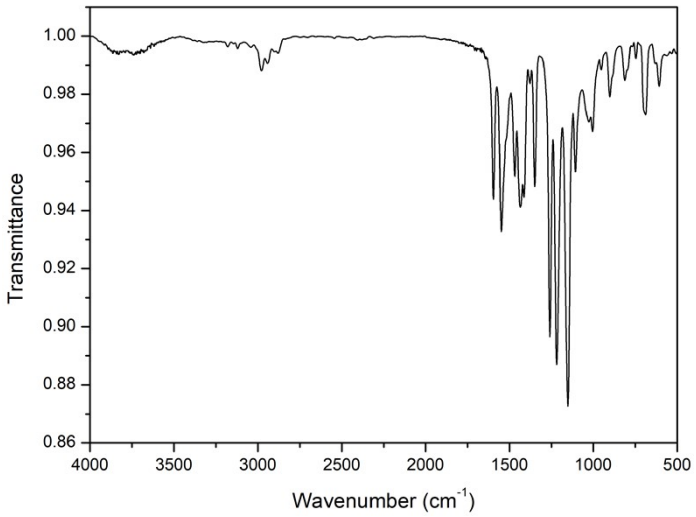

Fig S1-3. IR spectra of compound **3**.

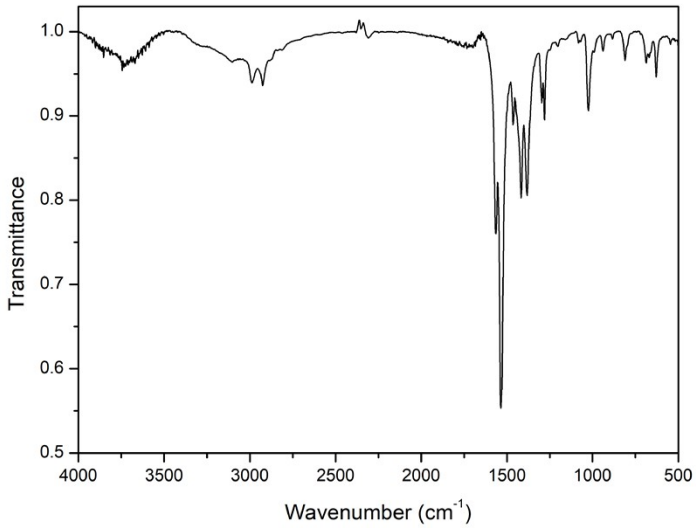

Fig S1-4. IR spectra of compound **4**.

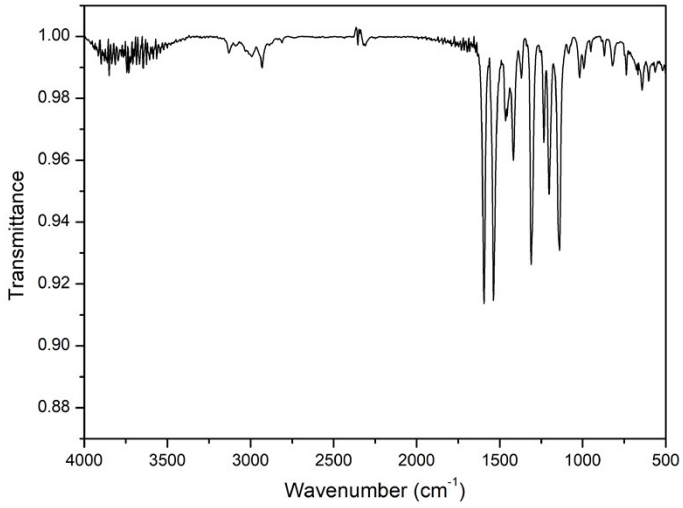

Fig S1-5. IR spectra of compound **5**.

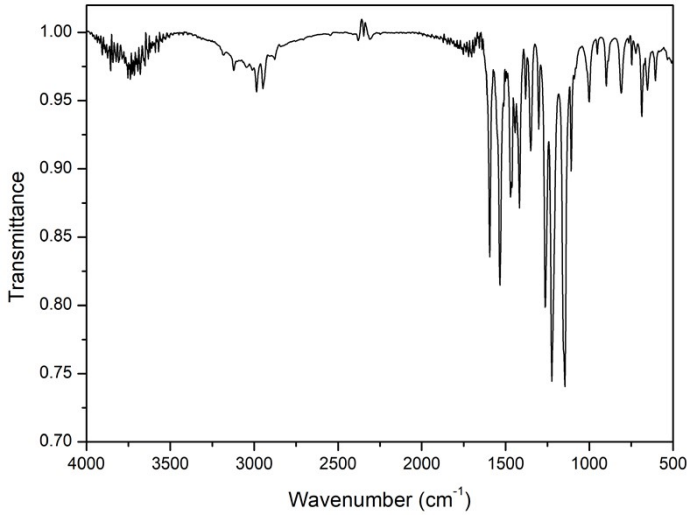

Fig S1-6. IR spectra of compound **6**.

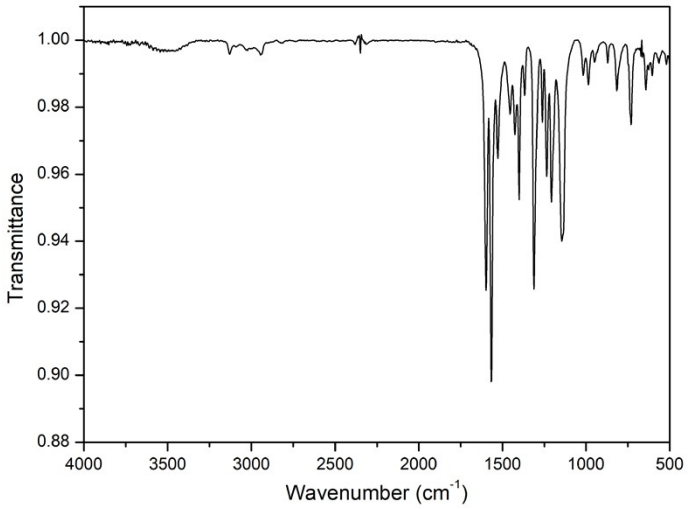

Fig S1-7. IR spectra of compound **7**.

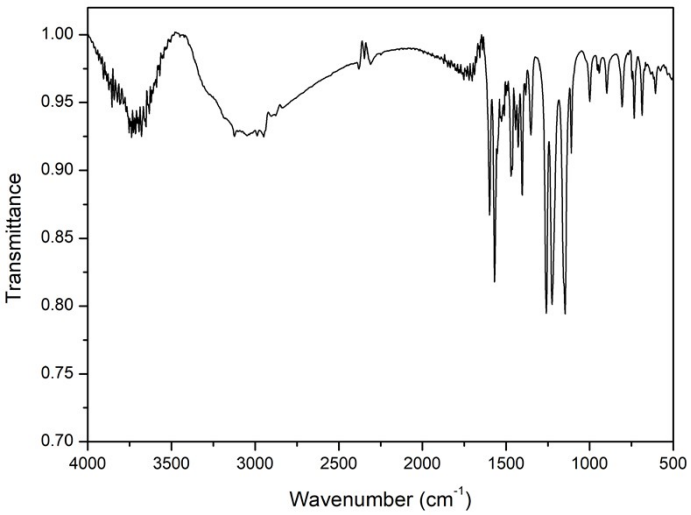

Fig S1-8. IR spectra of compound **8**.

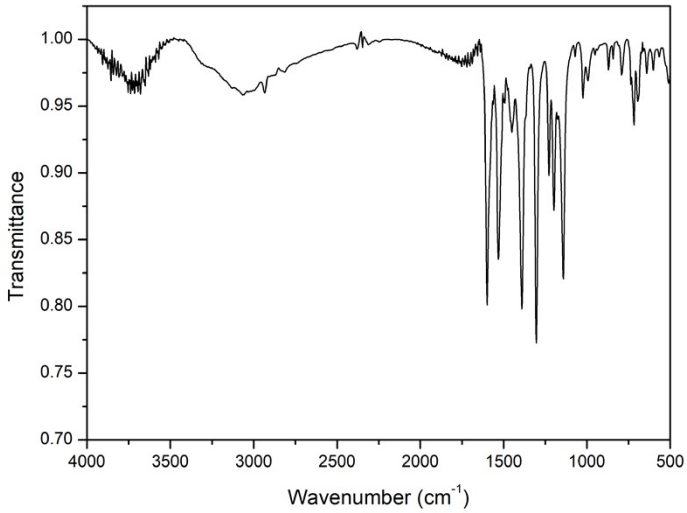

Fig S1-9. IR spectra of compound **9**.

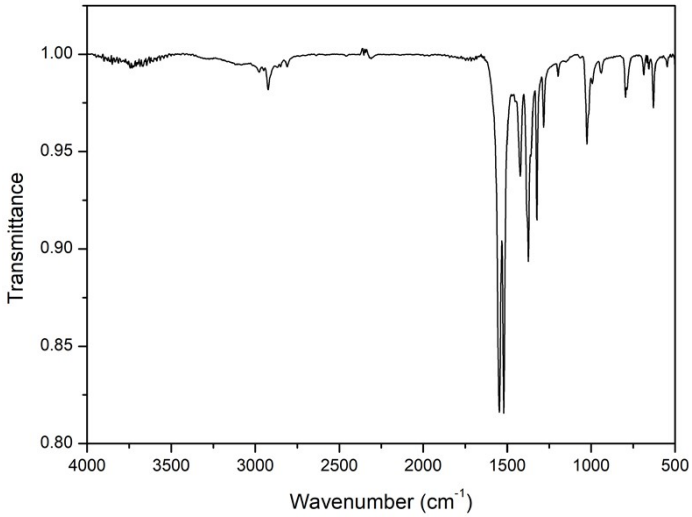

Fig S1-10. IR spectra of compound **10**.

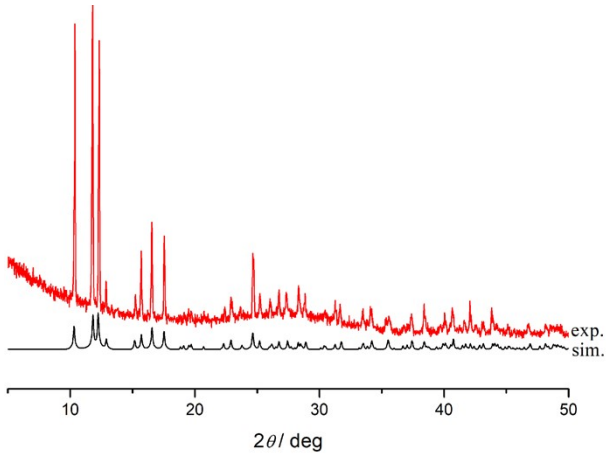

Fig. S2-1 Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and as-synthesized product of **1.**

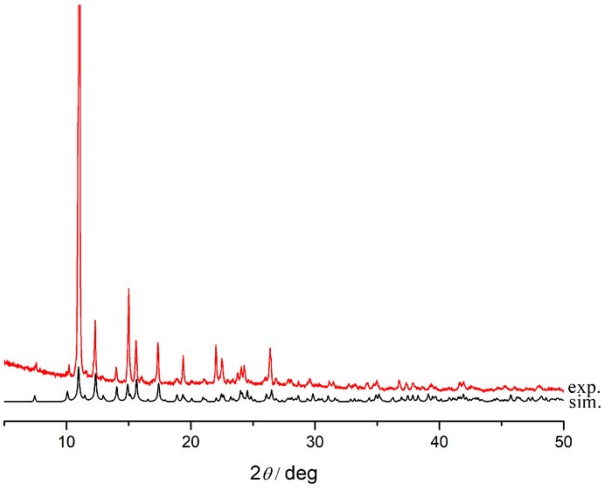

Fig. S2-2 Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and as-synthesized product of **2**.

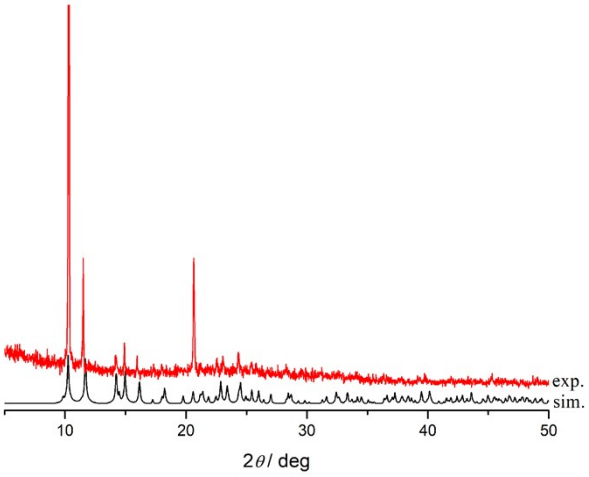

Fig. S2-3 Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and as-synthesized product of **3**

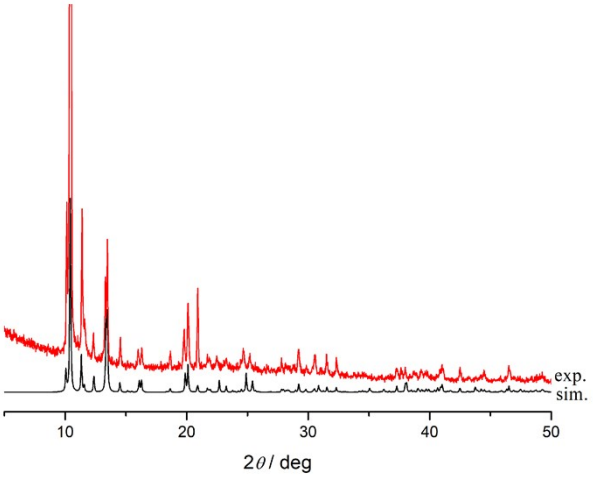

Fig. S2-4 Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and as-synthesized product of **4.**

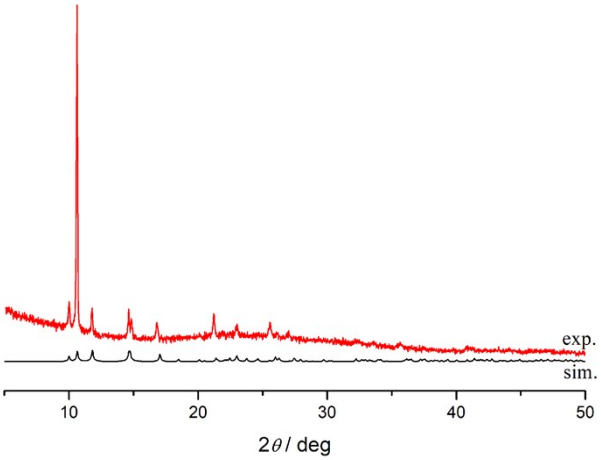

Fig. S2-5 Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and as-synthesized product of **5.**

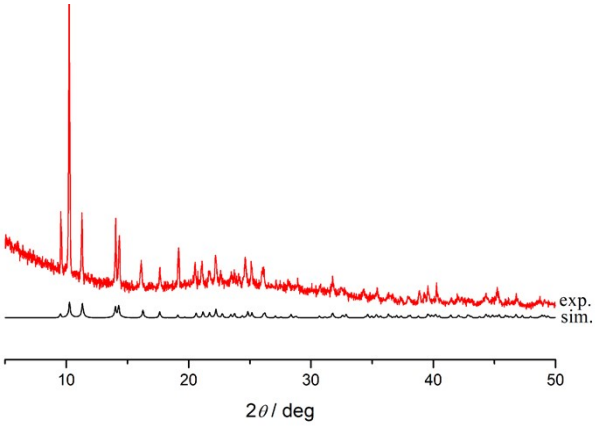

Fig. S2-6 Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and as-synthesized product of **6.**

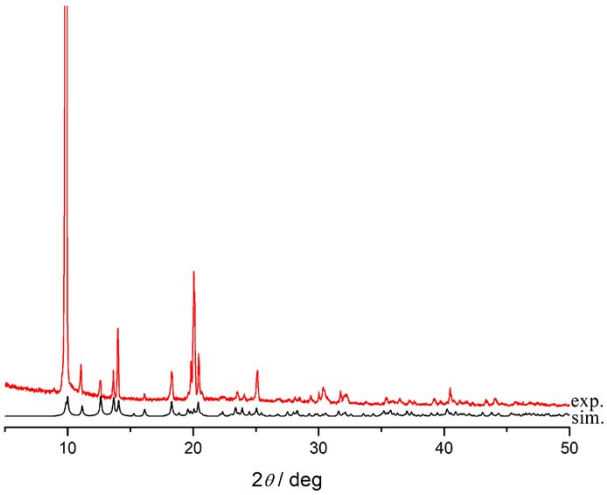

Fig. S2-7 Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and as-synthesized product of **7.**

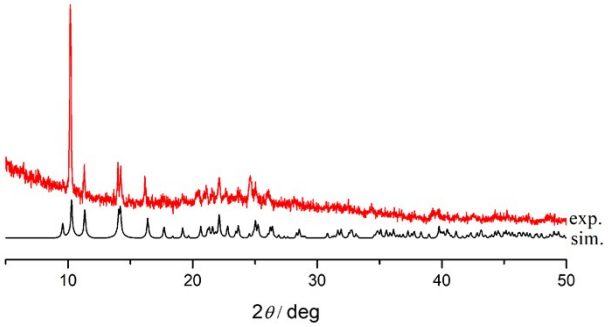

Fig. S2-8 Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and as-synthesized product of **8.**

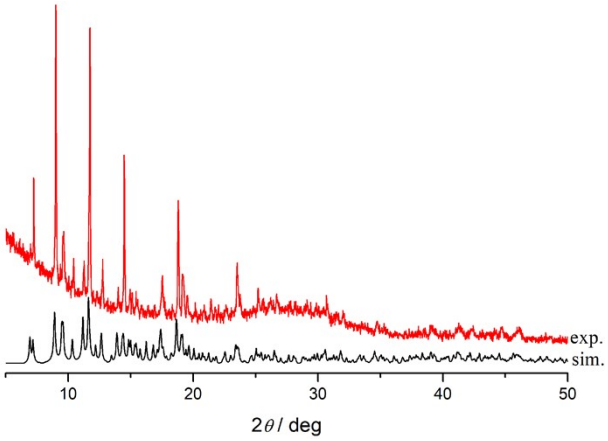

Fig. S2-9 Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and as-synthesized product of **9.**

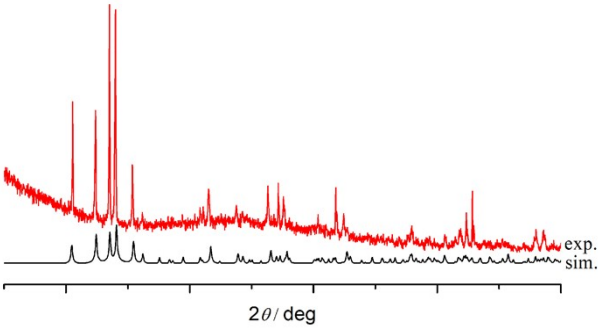

Fig. S2-10 Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and as-synthesized product of **10.**

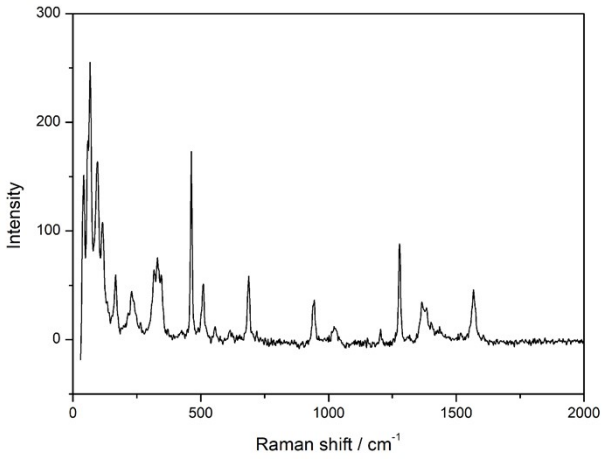

Fig. S3-1 Raman spectrum of compound **1.**

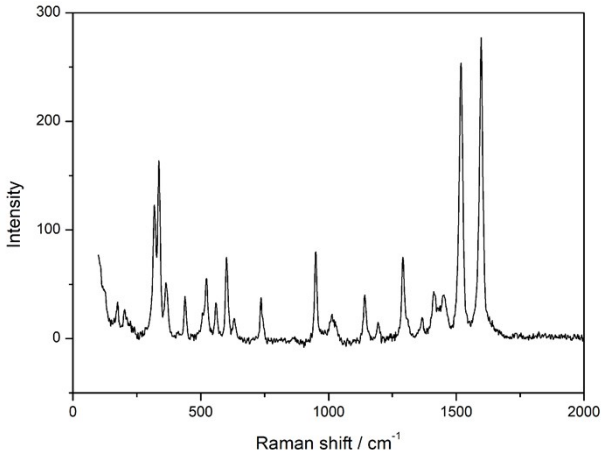

Fig. S3-2 Raman spectrum of compound **2**.

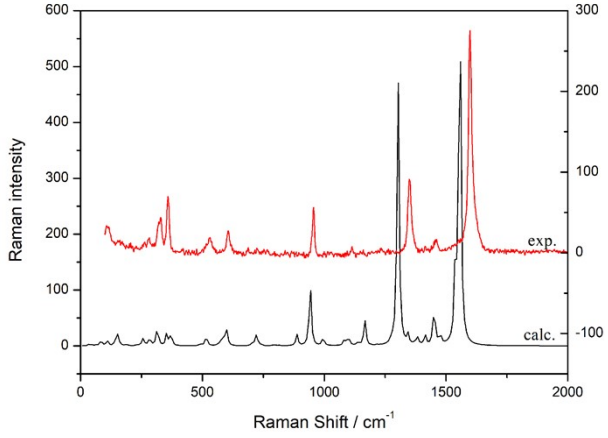

Fig. S3-3 Raman spectrum of compound **3**

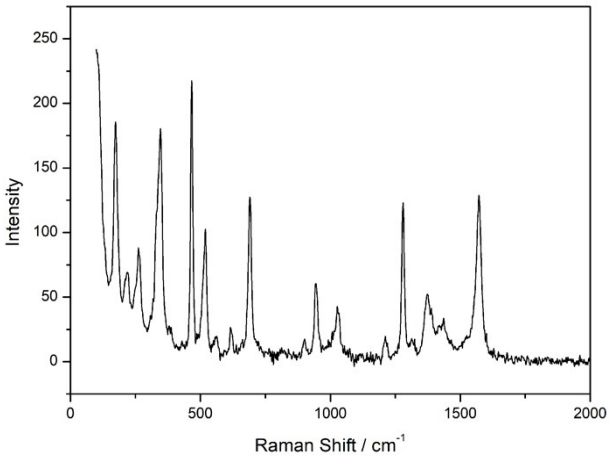

Fig. S3-4 Raman spectrum of compound **4**

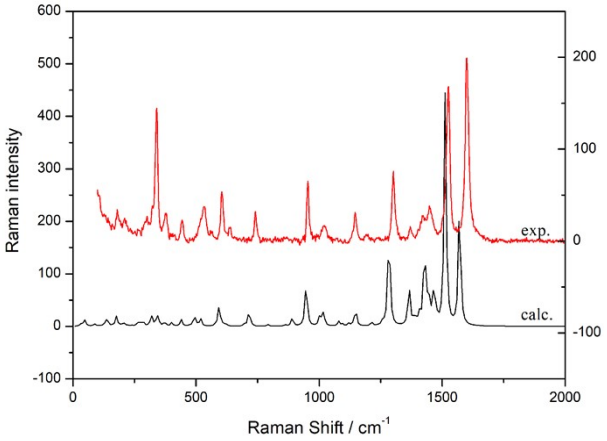

Fig. S3-5 Raman spectrum of compound **5**

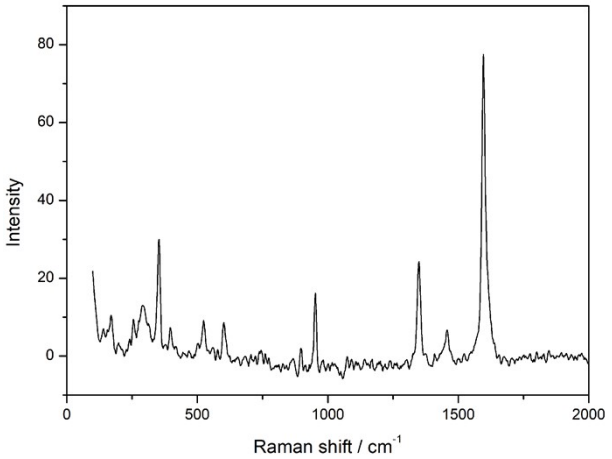

Fig. S3-6 Raman spectrum of compound **6**

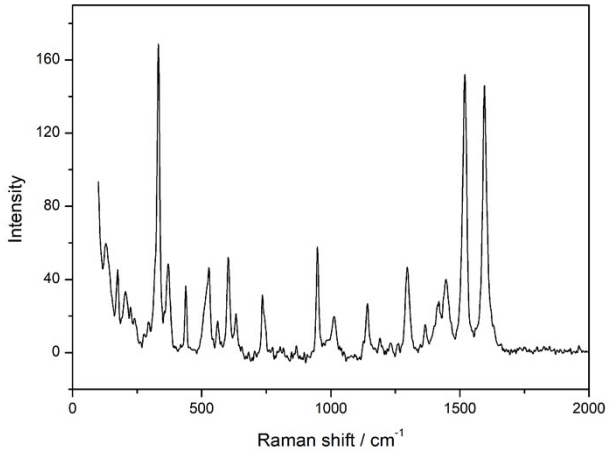

Fig. S3-7 Raman spectrum of compound **7**

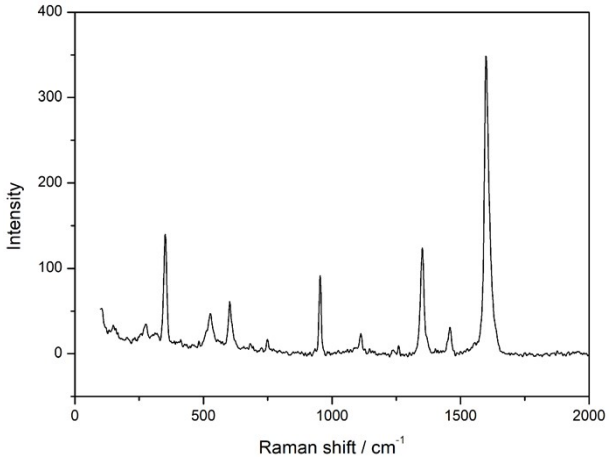

Fig. S3-8 Raman spectrum of compound **8**

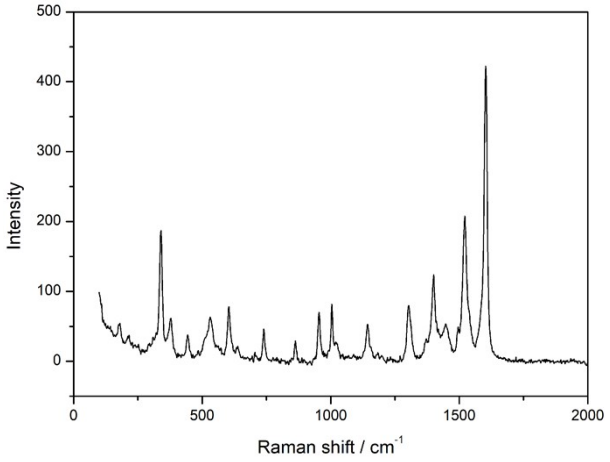

Fig. S3-9 Raman spectrum of compound **9**

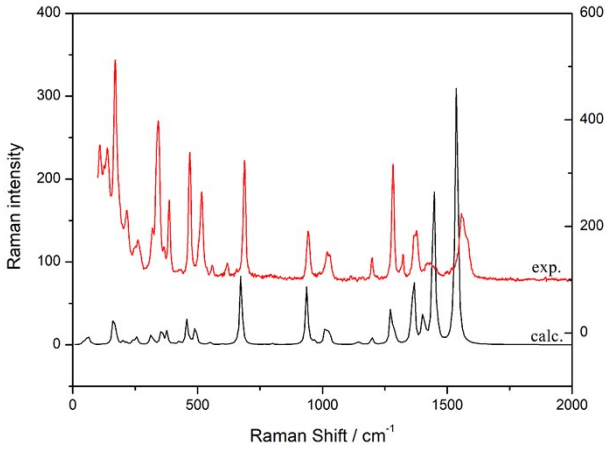

Fig. S3-10 Raman spectrum of compound **10**

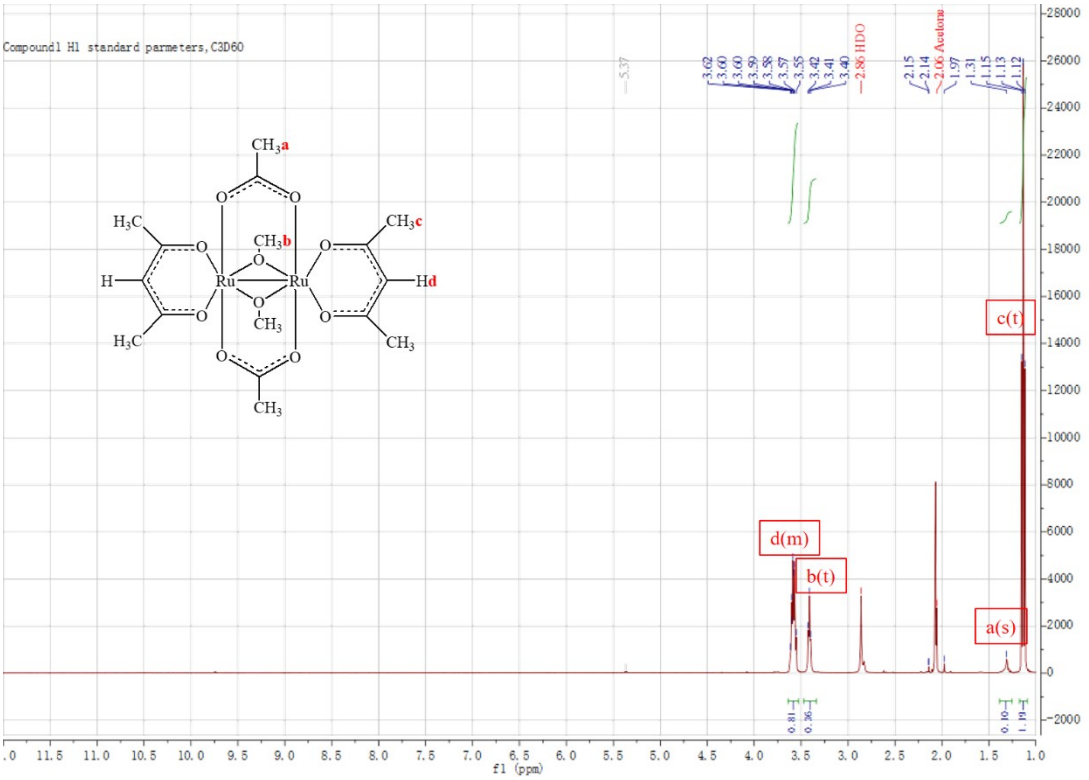

Fig. S4-1 ^{1}H NMR of **1** in $CDCl_3$ at 293 K.

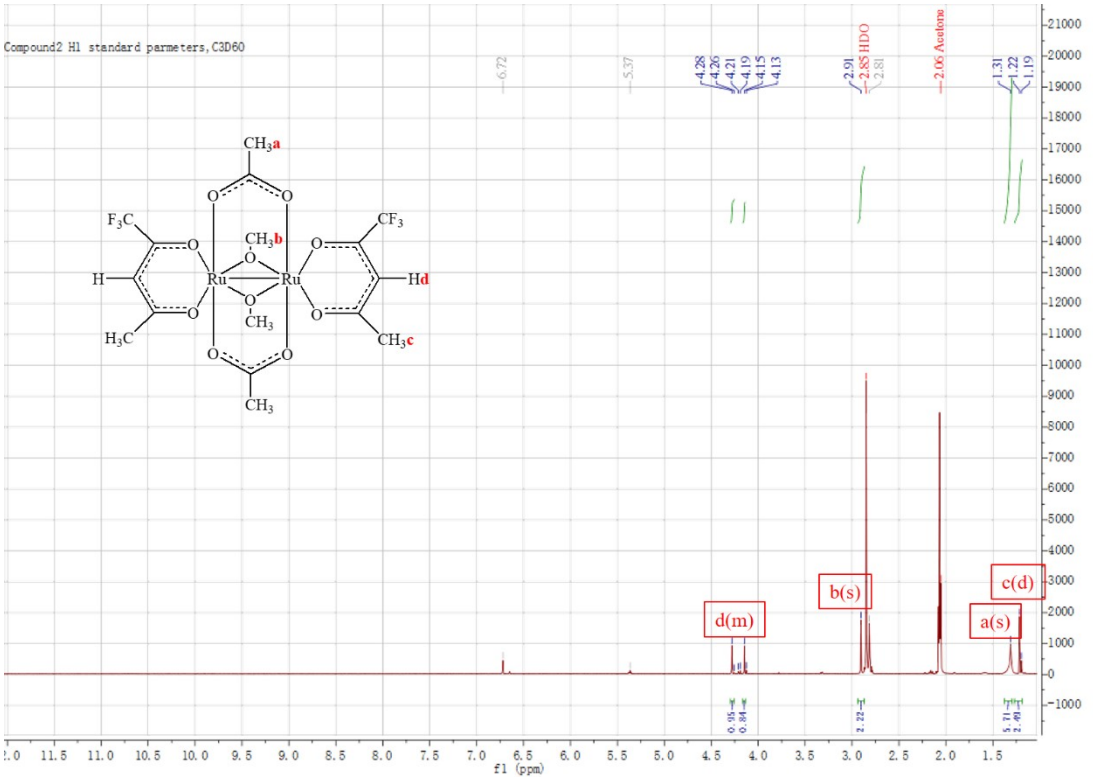

Fig. S4-2 ^{1}H NMR of **2** in $CDCl_3$ at 293 K.

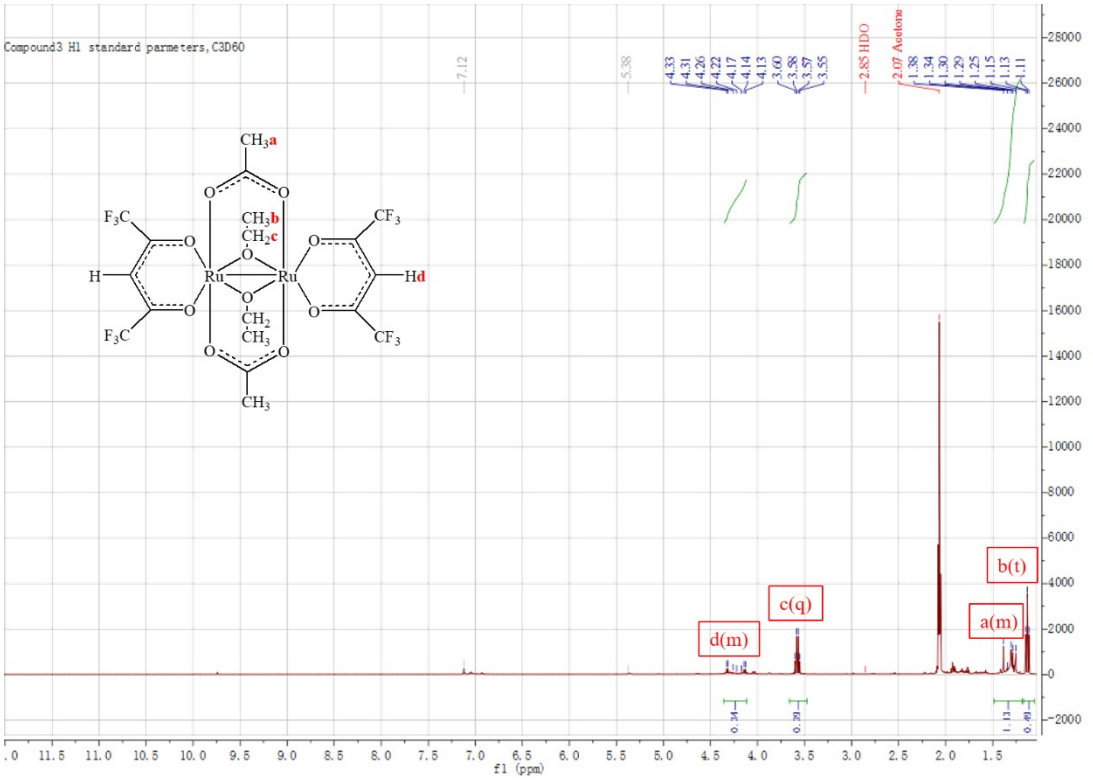

Fig. S4-3 ^{1}H NMR of **3** in $CDCl_3$ at 293 K.

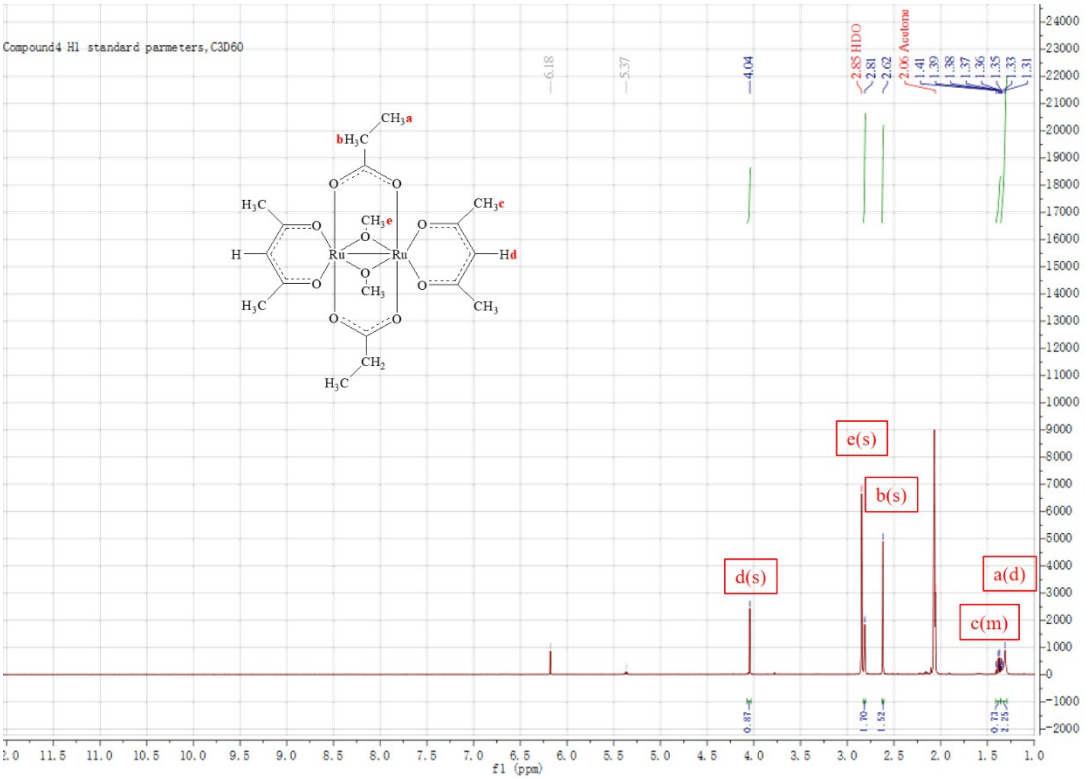

Fig. S4-4 ^{1}H NMR of **4** in $CDCl_3$ at 293 K.

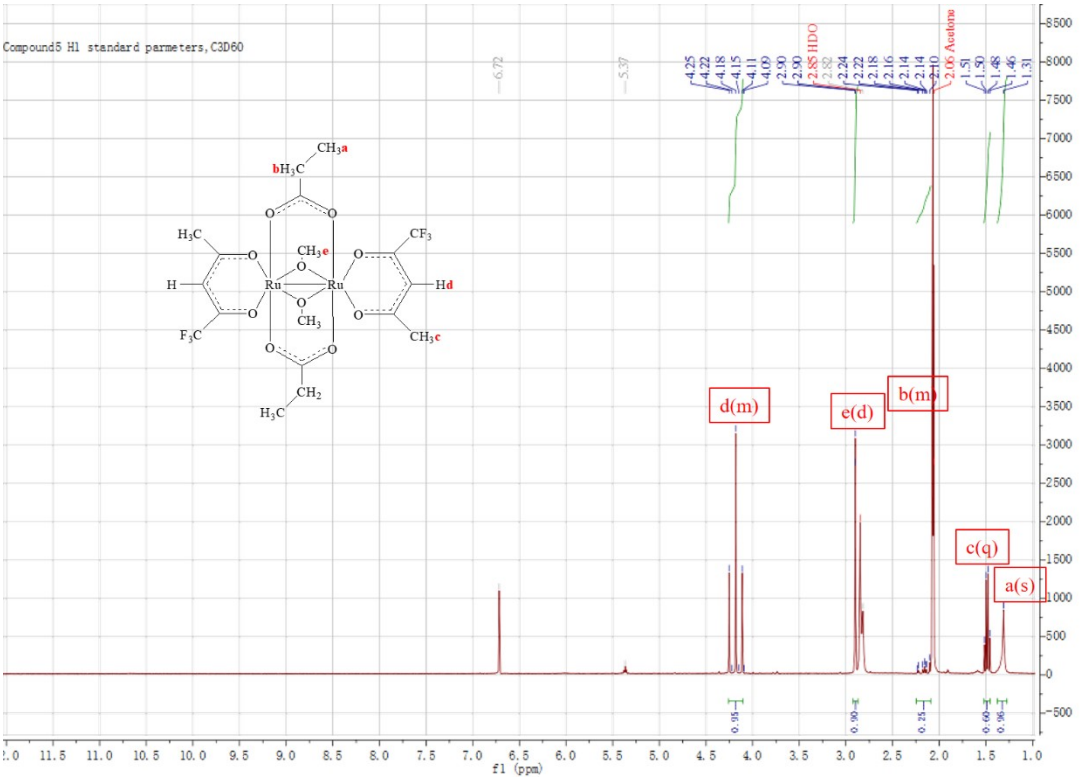

Fig. S4-5 ^{1}H NMR of **5** in $CDCl_3$ at 293 K.

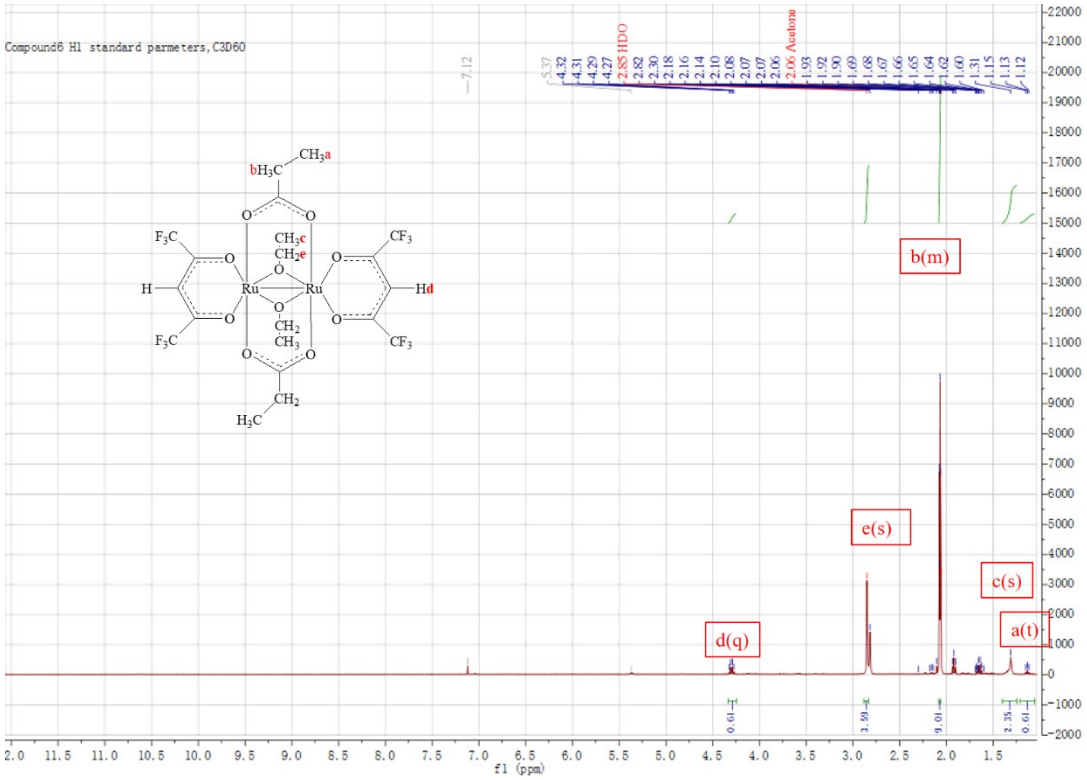

Fig. S4-6 ^{1}H NMR of **6** in $CDCl_3$ at 293 K.

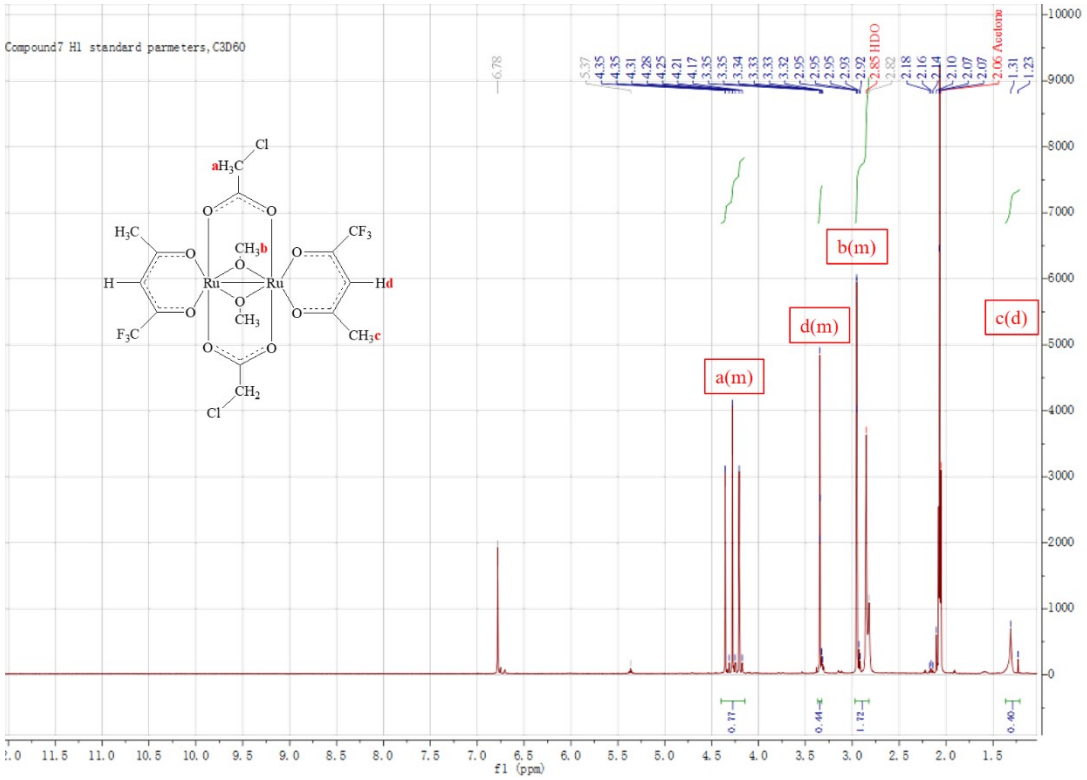

Fig. S4-7 ^{1}H NMR of **7** in $CDCl_3$ at 293 K.

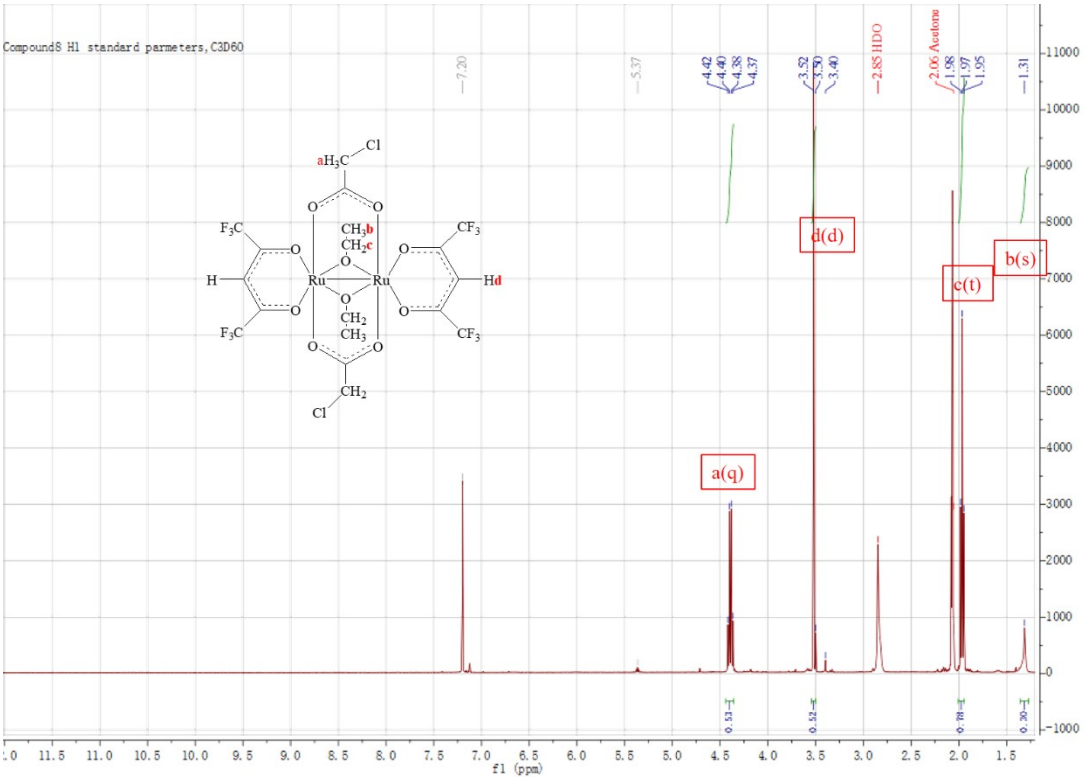

Fig. S4-8 ^{1}H NMR of **8** in $CDCl_3$ at 293 K.

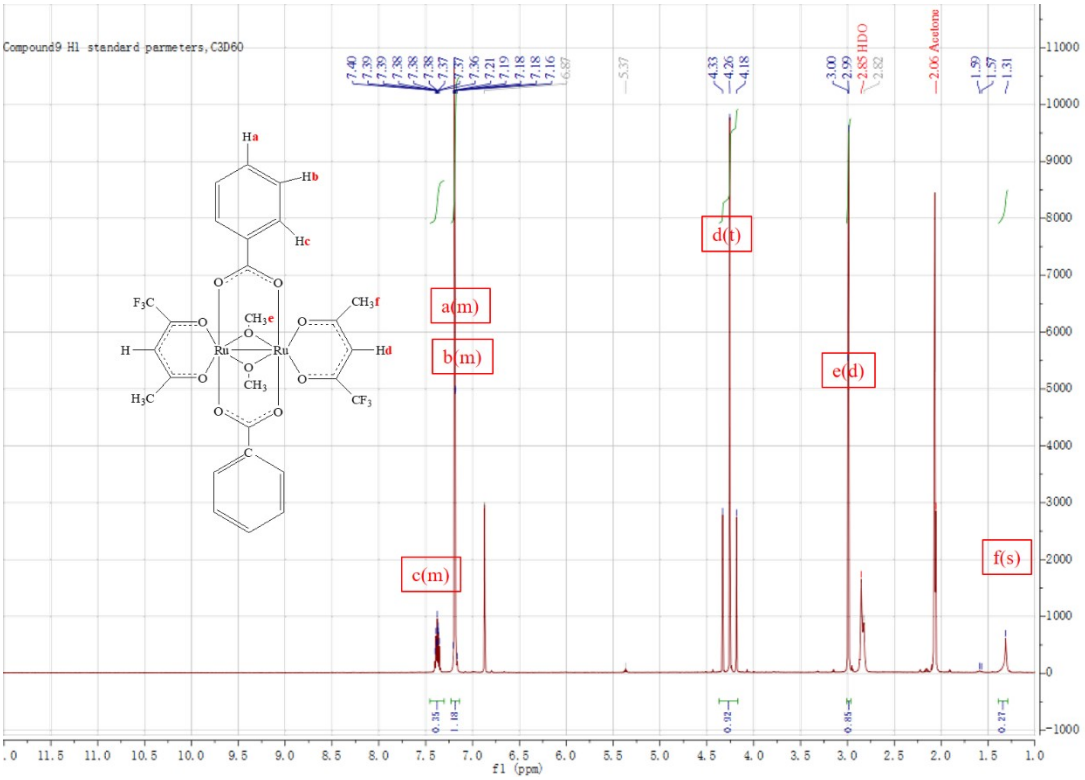

Fig. S4-9 ^{1}H NMR of **9** in $CDCl_3$ at 293 K.

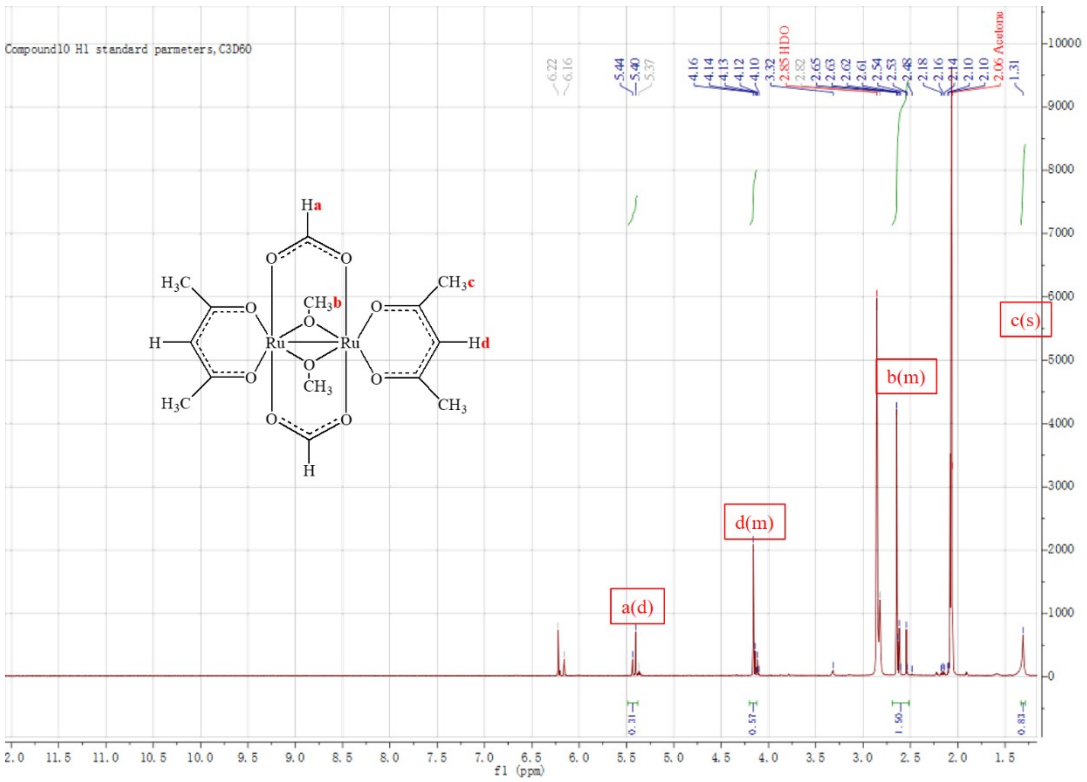

Fig. S4-10 ^{1}H NMR of **10** in $CDCl_3$ at 293 K.

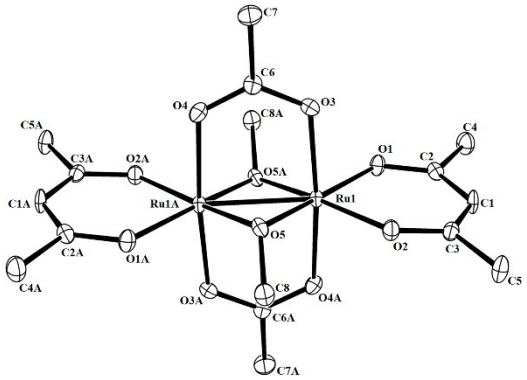

Fig. S5-1 ORTEP representation of the crystal structure of **1**

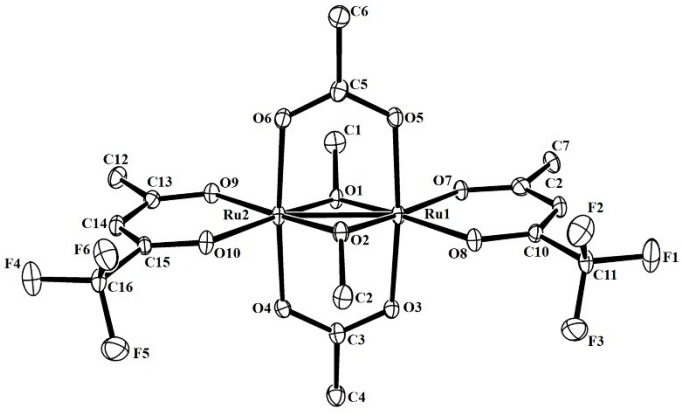

Fig. S5-2 ORTEP representation of the crystal structure of **2**

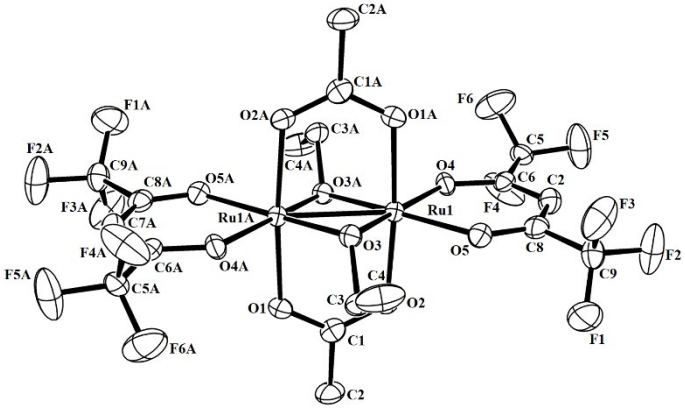

Fig. S5-3 ORTEP representation of the crystal structure of **3**

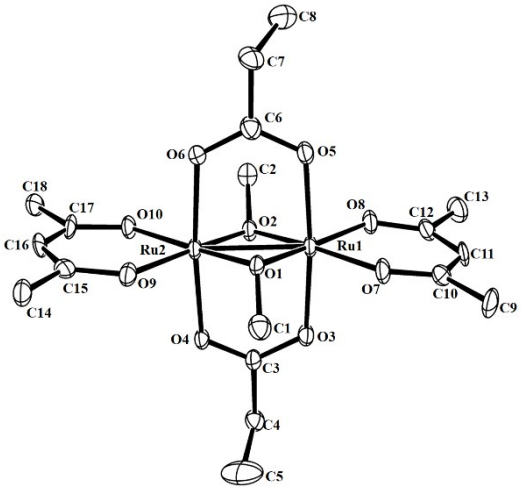

Fig. S5-4 ORTEP representation of the crystal structure of **4**

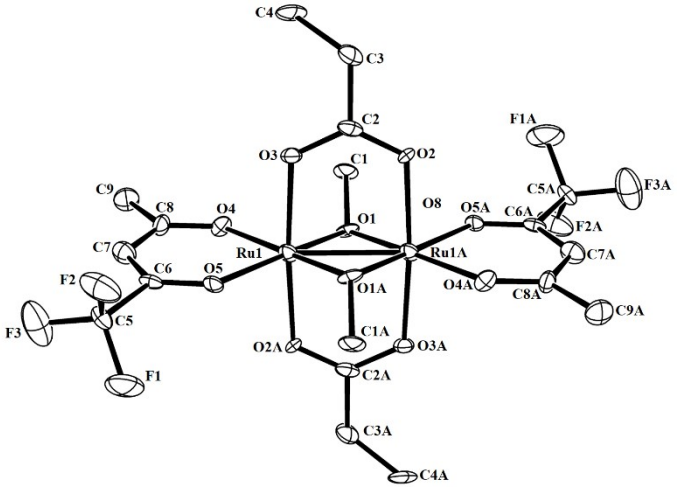

Fig. S5-5 ORTEP representation of the crystal structure of **5**

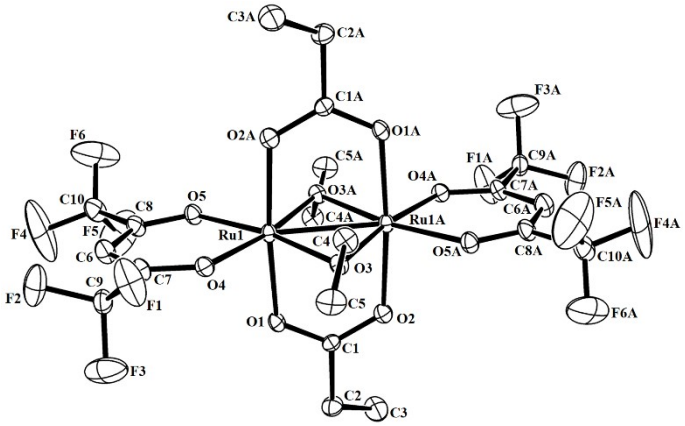

Fig. S5-6 ORTEP representation of the crystal structure of **6**

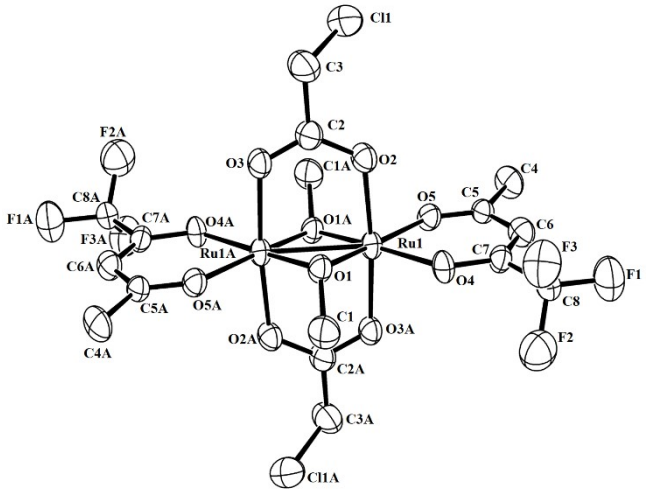

Fig. S5-7 ORTEP representation of the crystal structure of **7**

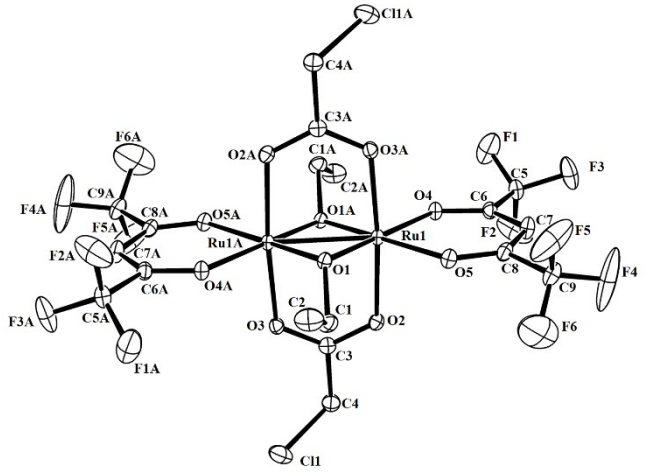

Fig. S5-8 ORTEP representation of the crystal structure of **8**

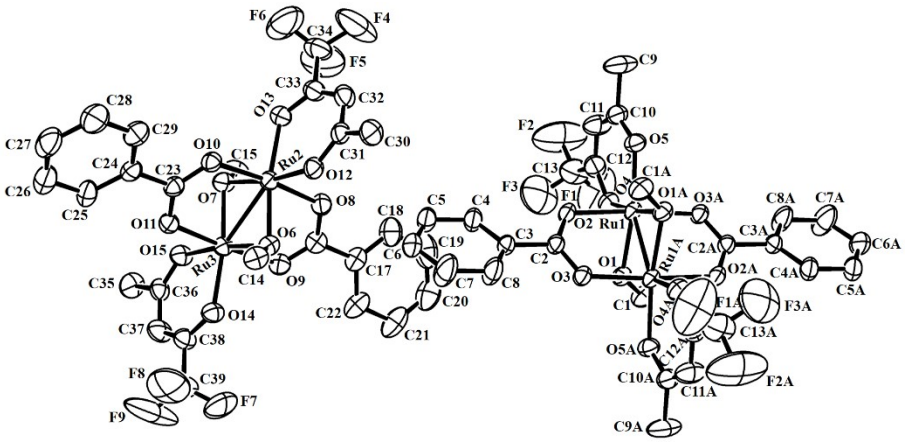

Fig. S5-9 ORTEP representation of the crystal structure of **9**

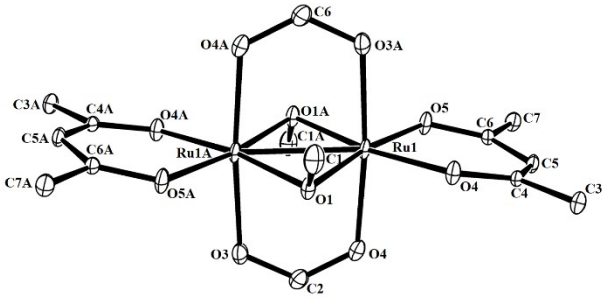

Fig. S5-10 ORTEP representation of the crystal structure of **10**

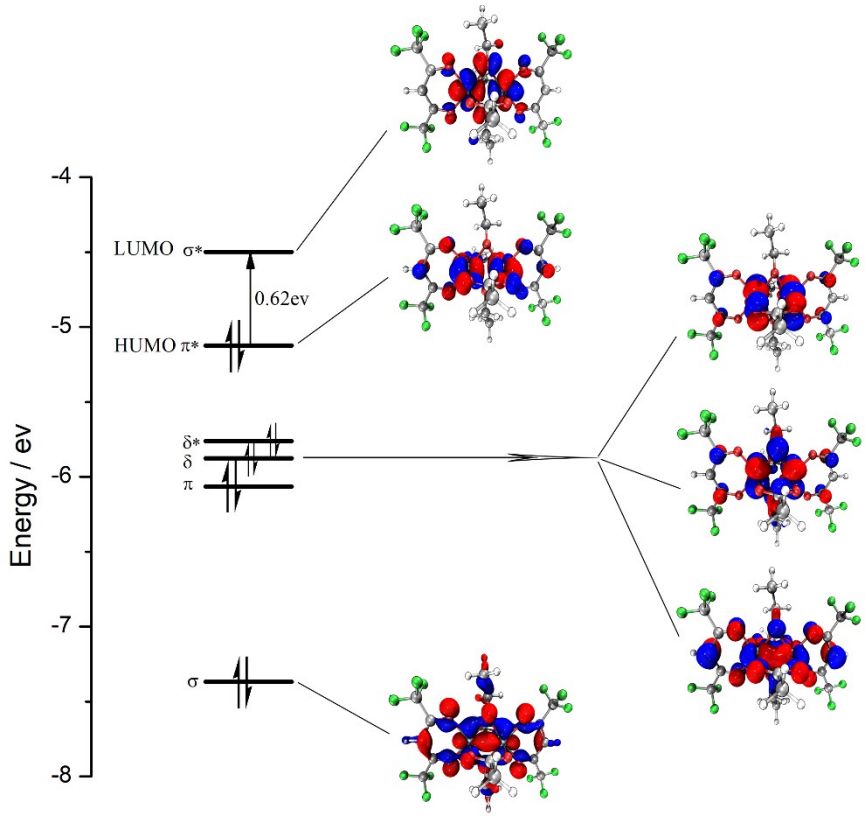

Fig S6-1. Molecular orbital diagrams of **3** with corresponding energies (eV)

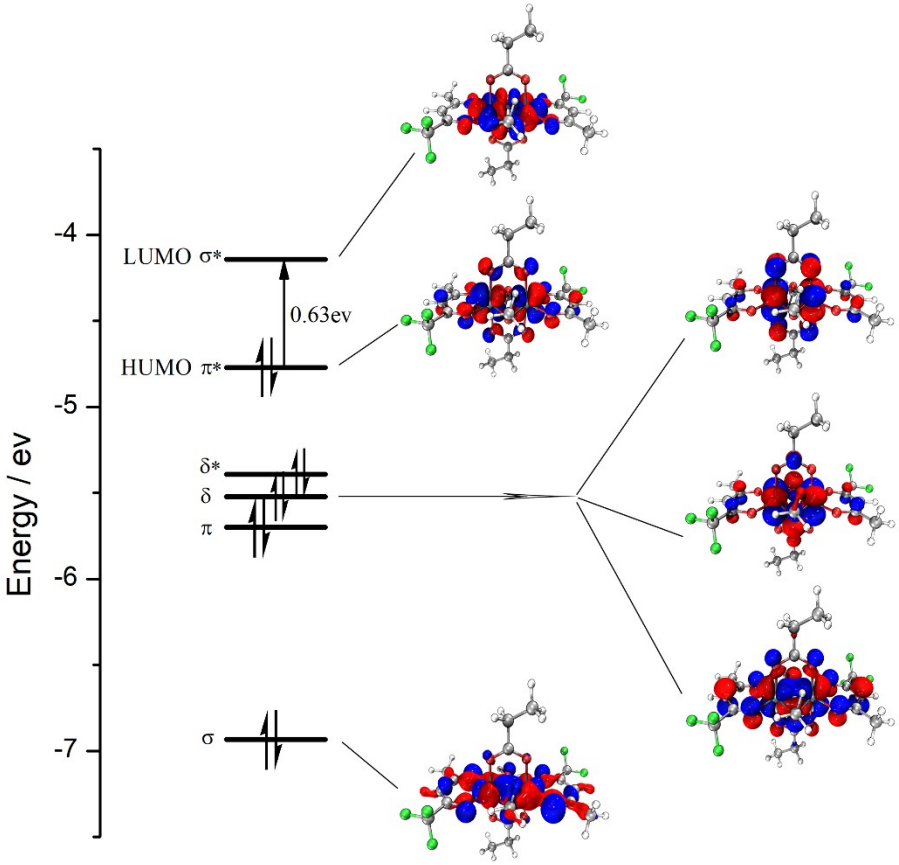

Fig S6-2. Molecular orbital diagrams of **5** with corresponding energies (eV)

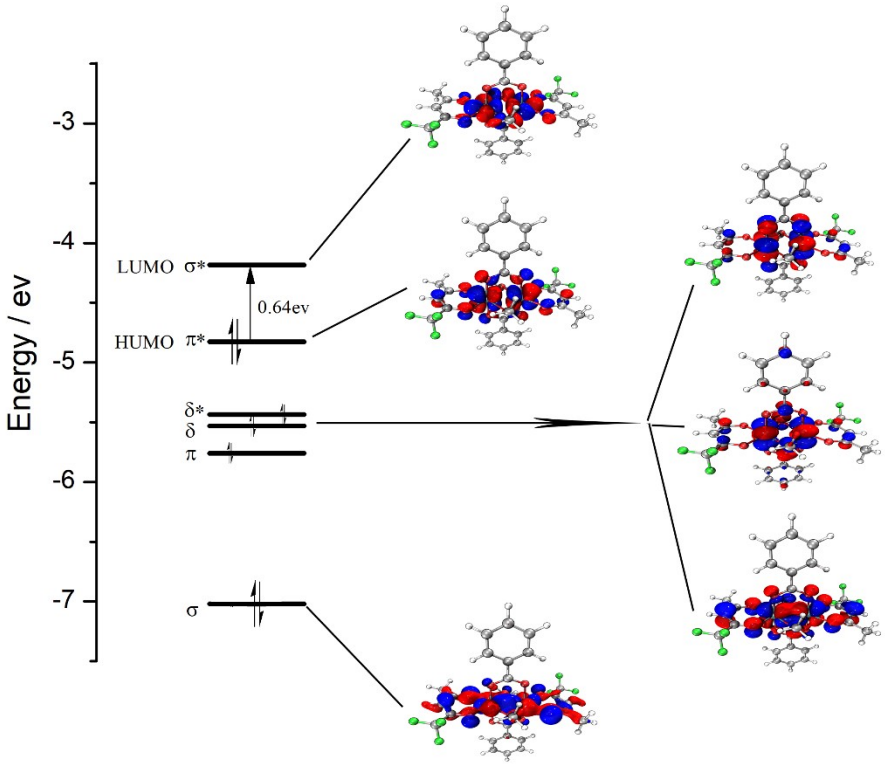

Fig S6-3. Molecular orbital diagrams of **9** with corresponding energies (eV)

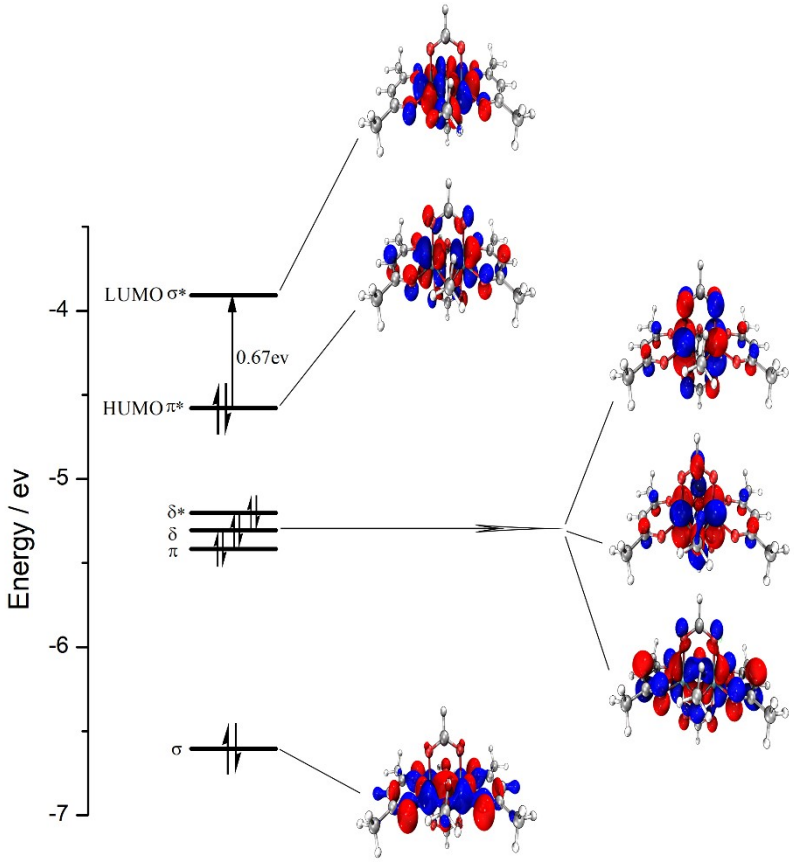

Fig S6-4. Molecular orbital diagrams of **10** with corresponding energies (eV)

Table S3-1. Selected bond distances (Å) from the experiment and calculation of compound **1**

	Exp.	Calc.
Ru(1)-O(5)A	1.998(5)	2.04976
Ru(1)-O(1)	2.021(5)	2.03610
Ru(1)-O(2)	2.020(5)	2.03610
Ru(1)-O(3)	2.081(5)	2.11362
Ru(1)-O(4)A	2.080(5)	2.11362
Ru(1)-Ru(1)A	2.476(2)	2.52291

Table S3-2. Selected bond distances (Å) from the experiment and calculation of compound **3**

	Exp.	Calc.
Ru(1)-O(3)A	1.991(6)	2.03505
Ru(1)-O(4)	2.026(6)	2.03582
Ru(1)-O(5)	2.030(6)	2.03423
Ru(1)-O(1)	2.065(7)	2.10904
Ru(1)-O(2)	2.073(7)	2.10487
Ru(1)-Ru(1)A	2.4560(9)	2.50669

Table S3-3. Selected bond distances (Å) from the experiment and calculation of compound **5**

	Exp.	Calc.

Ru(1)-O(1)A	1.978(10)	2.04759
Ru(1)-O(4)	2.009(10)	2.03554
Ru(1)-O(5)	2.024(10)	2.03450
Ru(1)-O(2)A	2.067(9)	2.10874
Ru(1)-O(3)	2.081(10)	2.11228
Ru(1)-Ru(1)A	2.450(6)	2.51591

Table S3-4. Selected bond distances (Å) from the experiment and calculation of compound **9**

	Exp.	Calc.
Ru(1)-O(1)A	1.991(4)	2.04339
Ru(1)-O(5)	2.019(4)	2.03577
Ru(1)-O(4)	2.030(4)	2.0349
Ru(1)-O(2)	2.065(4)	2.10973
Ru(1)-O(3)A	2.079(4)	2.09795
Ru(1)-Ru(1)A	2.4650(10)	2.51502

Table S3-5. Selected bond distances (Å) from the experiment and calculation of compound **10**

	Exp.	Calc.
Ru(1)-O(1)A	1.999(2)	2.04951
Ru(1)-O(5)	2.013(2)	2.03528
Ru(1)-O(4)	2.022(3)	2.03467
Ru(1)-O(3)A	2.077(2)	2.11932
Ru(1)-O(2)	2.086(2)	2.12349
Ru(1)-Ru(1)A	2.4771(4)	2.53223

Table S4 Vibrational frequencies (ν, cm^{-1}) of compounds **3**, **5** and **10**. Experiment data are shown in bold, DFT-computed values in normal.

	ν(Ru-Ru)	ν(Ru-O_a)	ν(Ru-O_b)	ν(Ru-O_t)	ν(C-O)	ν(C-C)	ν(C-F/H)
3	**358**	**320**	**605**	**150**	**1597**	**1351**	**1598**
	364	305	574	145	1552	1298,1534	1448
5	**339**	**298**	**518**	**178**	**1599**	**1301,1525**	**539;1523**
	338	268	486	169	1566	1278,1507	511;1423
10	**341**	**386**	**513**	**167**	**1557**	**1283**	**674;1369**
	345	369	484	156	1533	1269	667;1442

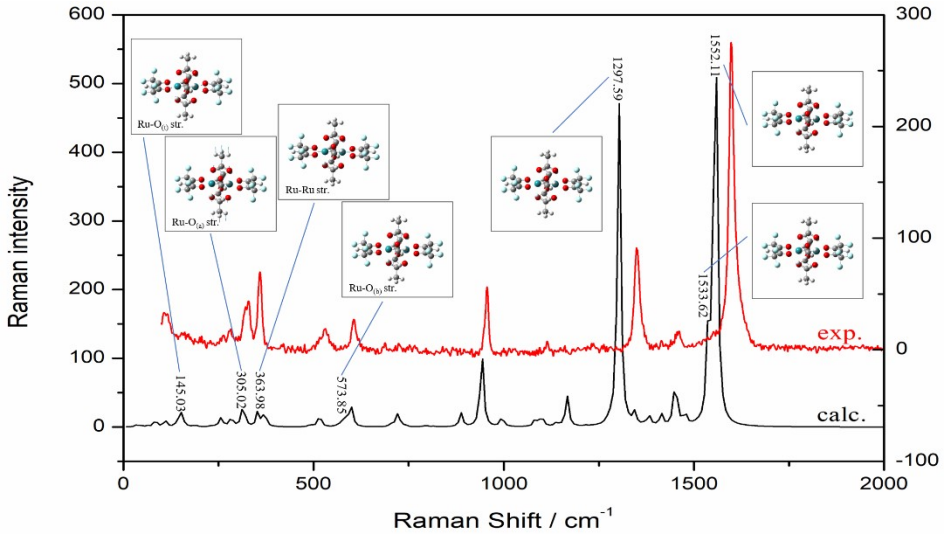

Fig. S7-1 Experimental and calculated raman spectra for compound **3** (hfac).

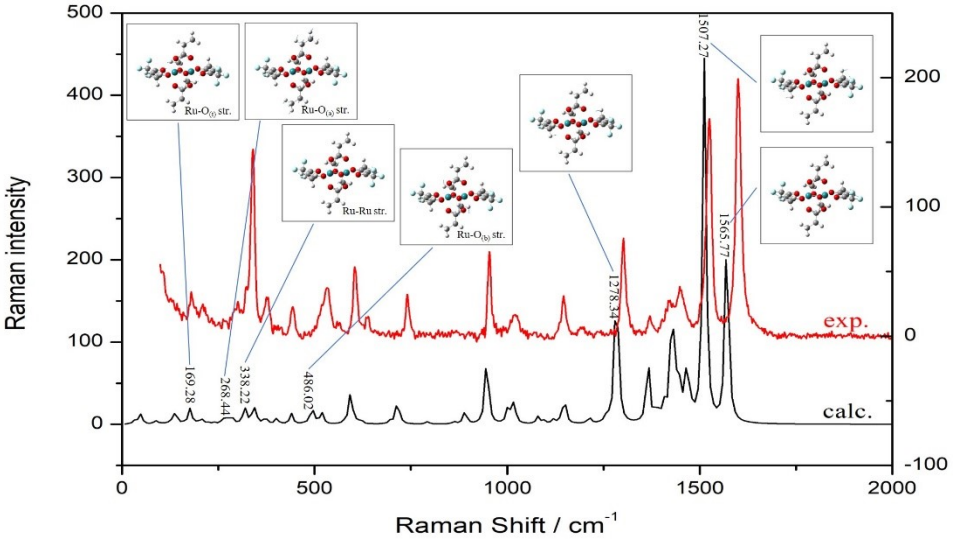

Fig. S7-2 Experimental and calculated raman spectra for compound **5** (tfac).

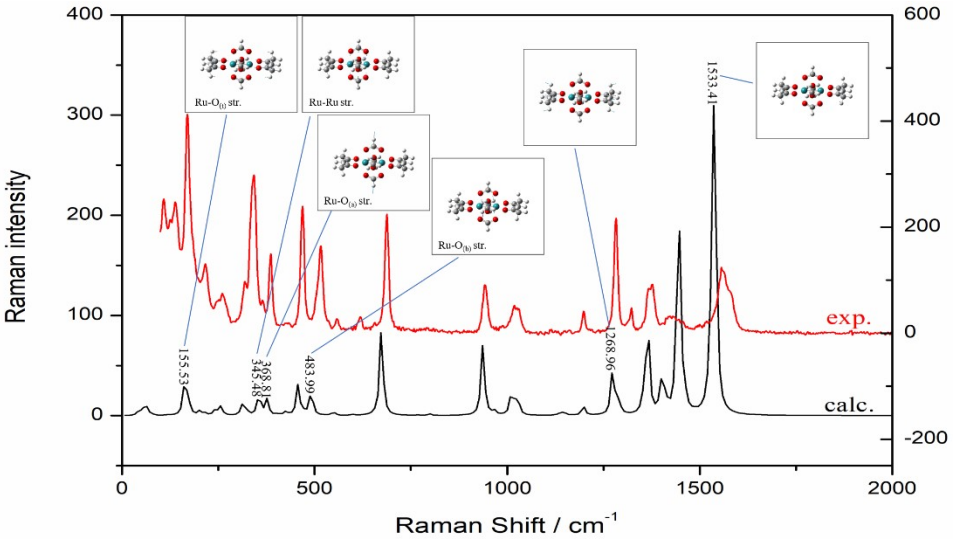

Fig. S7-3 Experimental and calculated raman spectra for compound **10** (acac).

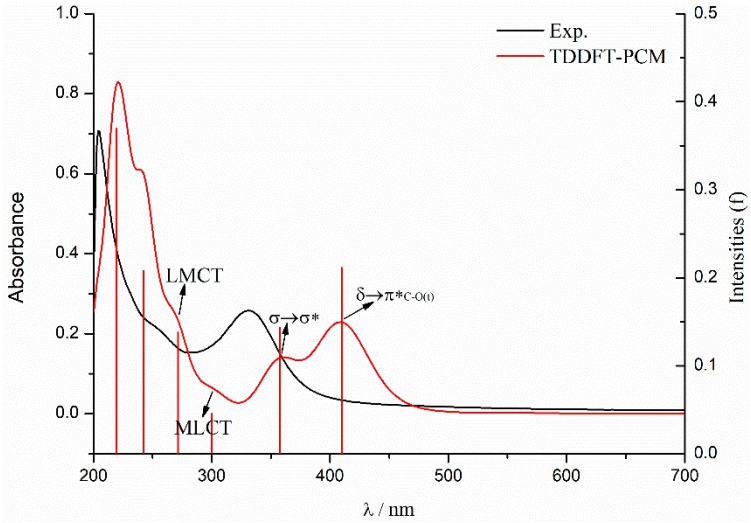

Fig. S8-1 Experimental and calculated UV–vis spectra for compound **1**.

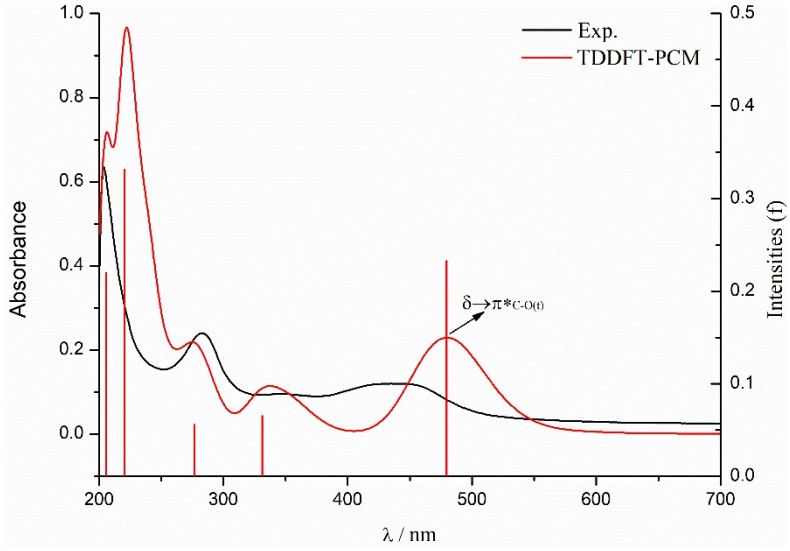

Fig. S8-2 Experimental and calculated UV–vis spectra for compound **3**.

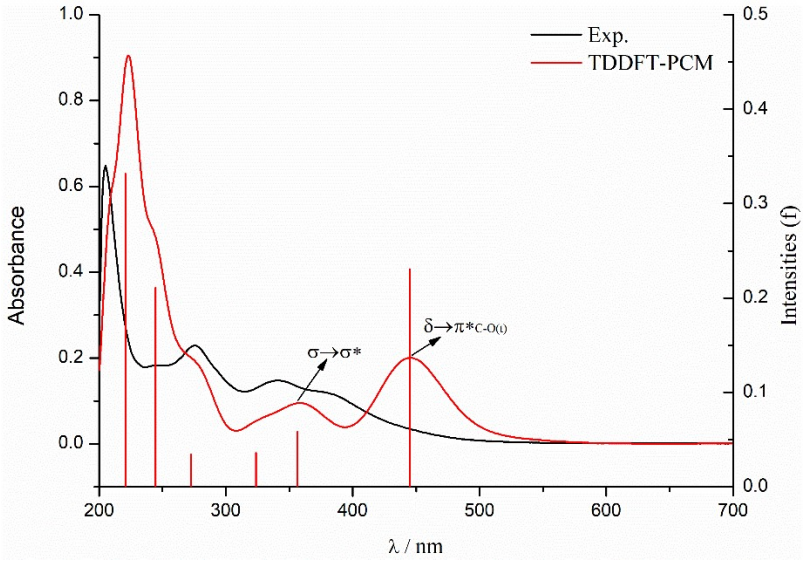

Fig. S8-3 Experimental and calculated UV–vis spectra for compound **5**.

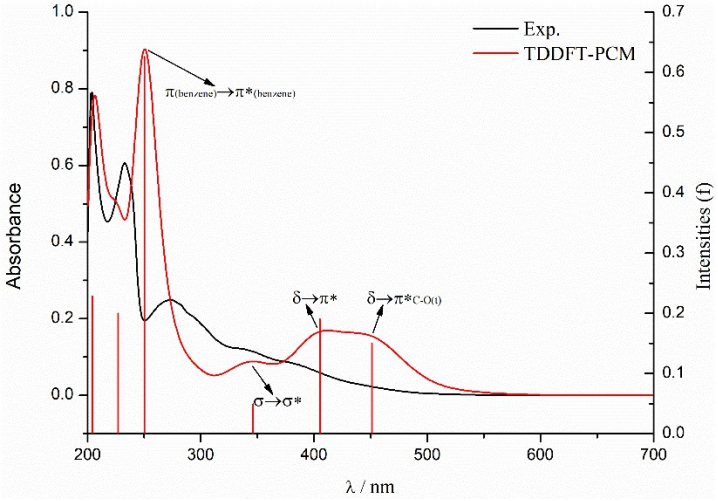

Fig. S8-4 Experimental and calculated UV–vis spectra for compound **9**.

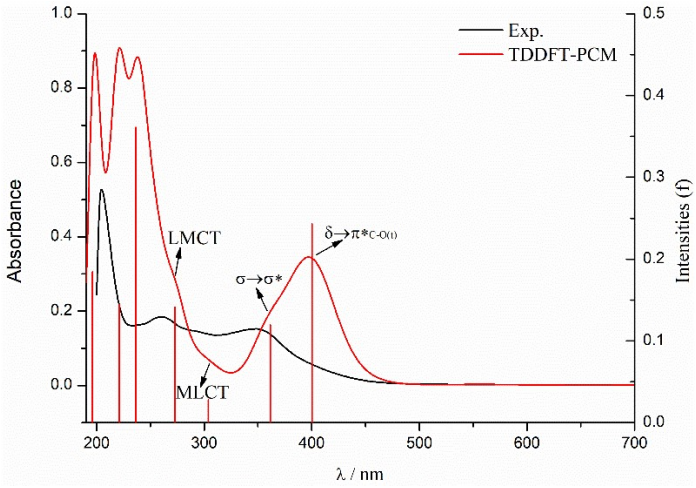

Fig. S8-5 Experimental and calculated UV–vis spectra for compound **10**.

Table S5-1 The representative calculated optical transitions for compound **1**

λ（nm）	f	assign.	%
409.67	0.2118	$\delta\rightarrow\pi^*_{C\text{-}O(t)}$	42
357.56	0.1432	$\sigma\rightarrow\sigma^*$	81
300.19	0.0460	$\delta\rightarrow\pi^*_{C\text{-}O(a)}$	96
271.43	0.1384	$P_{(C/O)}\rightarrow\pi^*$	69
242.38	0.2082	$\sigma_{Ru\text{-}O(a)}\rightarrow\pi^*_{C\text{-}O(t)}$	25
217.46	0.3695	$\sigma_{Ru\text{-}O(a)}\rightarrow\sigma^*_{Ru\text{-}O(a)}$	31

Table S5-2. The representative calculated optical transitions for compound **3**

λ（nm）	f	assign.	%
479.66	0.2326	$\delta\rightarrow\pi^*_{C\text{-}O(t)}$	63
331.38	0.0656	$\sigma_{Ru\text{-}O(b)}\rightarrow\sigma^*$	54
276.61	0.0558	$\sigma_{Ru\text{-}O(a)}\rightarrow\sigma^*$	19
220.51	0.3315	$\sigma_{Ru\text{-}O}\rightarrow\sigma^*_{Ru\text{-}O(a)}$	12
202.68	0.2195	$\sigma_{Ru\text{-}O(a)}\rightarrow\sigma^*_{Ru\text{-}O(a)}$	12

Table S5-3 The representative calculated optical transitions for compound **5**

λ（nm）	f	assign.	%
444.78	0.2307	$\delta\rightarrow\pi^*_{C\text{-}O(t)}$	68
356.58	0.0587	$\sigma\rightarrow\sigma^*$	43
323.87	0.0361	$\sigma^*_{Ru\text{-}O(b)}\rightarrow\sigma^*$	89
272.65	0.0343	$\sigma\rightarrow\sigma^*_{Ru\text{-}O(t)}$	32
244.59	0.2110	$\sigma_{Ru\text{-}O(a)}\rightarrow\sigma^*_{Ru\text{-}O(t)}$)	17
220.81	0.3319	$\sigma_{Ru\text{-}O(a)}\rightarrow\sigma^*_{Ru\text{-}O(a)}$	12

Table S5-4. The representative calculated optical transitions for compound **9**

λ（nm）	f	assign.	%
451.22	0.1501	$\delta\rightarrow\pi^*_{C\text{-}O(t)}$	43
405.17	0.1906	$\delta\rightarrow\pi^*$	49
346.31	0.0495	$\sigma\rightarrow\sigma^*$	28
250.24	0.6262	$\pi_{(benzene)}\rightarrow\pi^*_{(benzene)}$	30
226.93	0.1998	$\sigma_{Ru\text{-}O(t)}\rightarrow\sigma^*_{Ru\text{-}O(t)}$)	27
204.30	0.2289	$\sigma_{Ru\text{-}O(b)}\rightarrow\sigma^*_{Ru\text{-}O(a)}$)	42

Table S5-5. The representative calculated optical transitions for compound **10**

λ（nm）	f	assign.	%
400.15	0.2433	$\delta\rightarrow\pi^*_{C\text{-}O(t)}$	61
361.42	0.1197	$\sigma\rightarrow\sigma^*$	71
303.96	0.0281	$\delta\rightarrow\pi^*_{C\text{-}O(a)}$	96
272.68	0.1408	$P_{(C/O)}\rightarrow\pi^*$	78
236.40	0.3611	$\sigma_{Ru\text{-}O(b)}\rightarrow\sigma^*_{Ru\text{-}O(a)}$	48
221.14	0.1446	$P_{(O)}\rightarrow\pi$	25
196.26	0.1844	$\sigma_{Ru\text{-}O}\rightarrow\pi$	29

Table S6 The differential pulse voltammograms (DPV) peaks data (E/V) for compounds **1-10**

	1	2	3	4	5	6	7	8	9	10
A	-0.58	-0.64	-0.62	-0.63	-0.62	-0.61	-0.61	-0.62	-0.61	-0.60
B	0.90	0.82	0.85	0.84	0.86	0.85	0.86	0.86	0.88	0.86
C	1.26	1.18	1.26	1.25	1.26	1.26	1.26	1.26	1.27	1.23