Supporting Information

for

Water Oxidation Catalyzed by Charge-neutral Mononuclear Ruthenium(III) Complex

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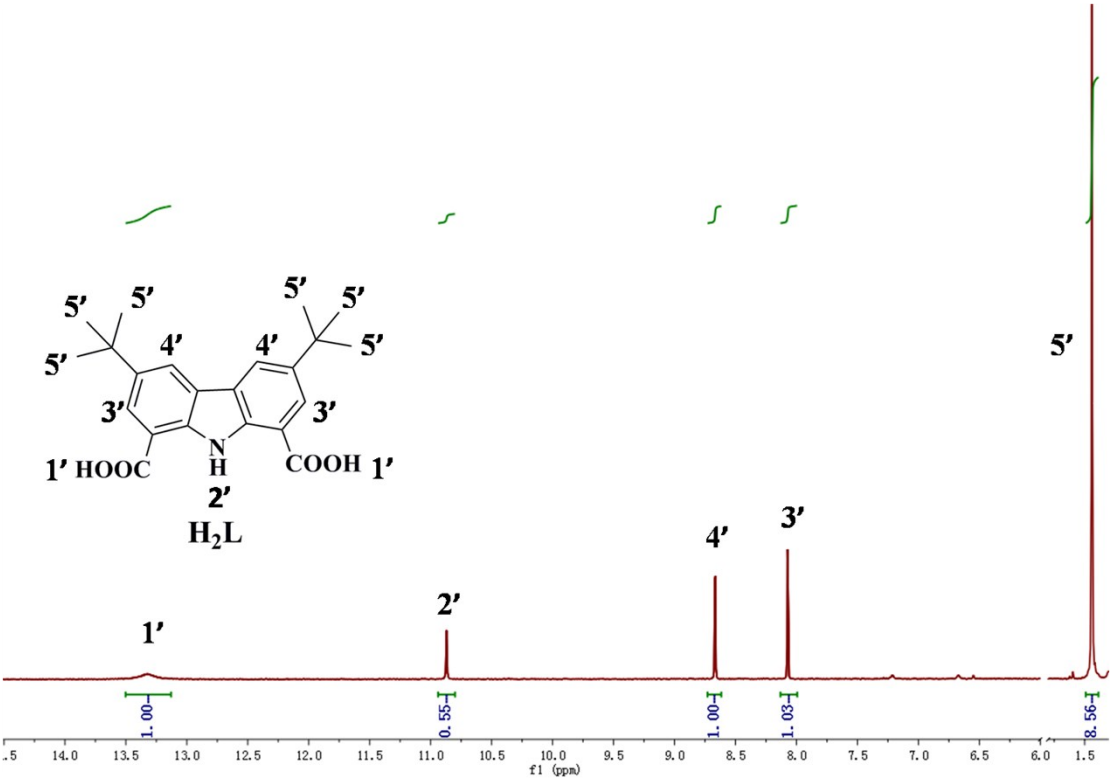

Figure S1. ^{1}H NMR of H_2L in d_6-DMSO.

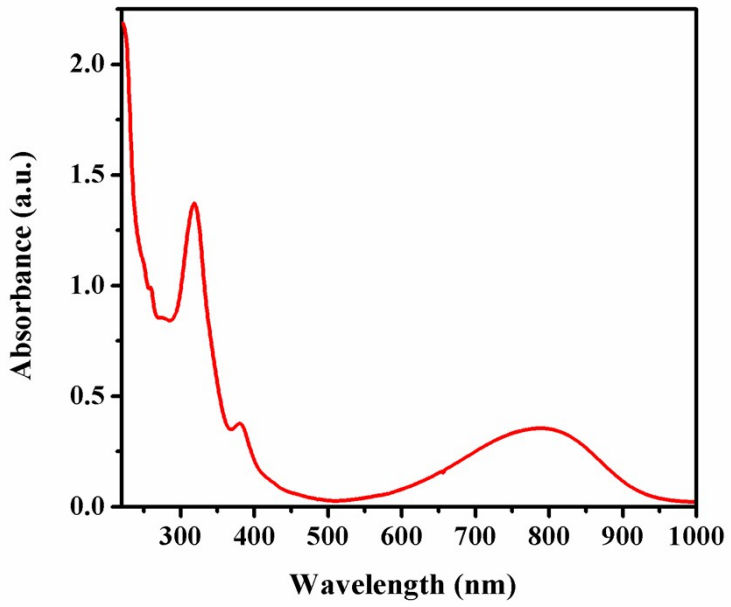

Figure S2. UV−vis. absorption spectra of **1** in CF_3CH_2OH solution.

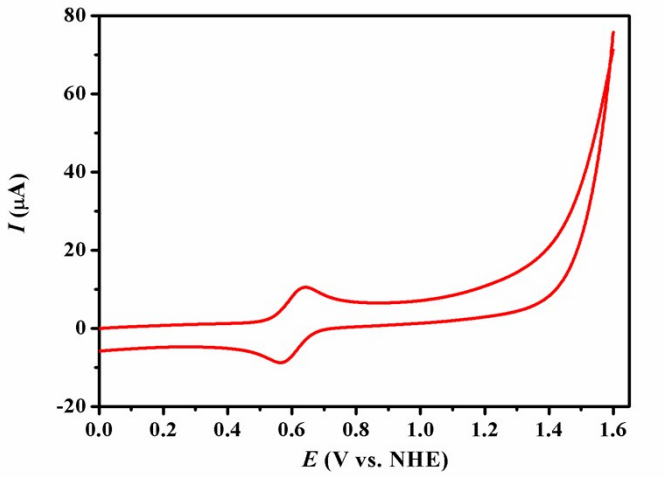

Figure S3. CV curve of **1** in pH 6.86 phosphate buffer containing 30% CF_3CH_2OH (scan rate = 100 mV/s).

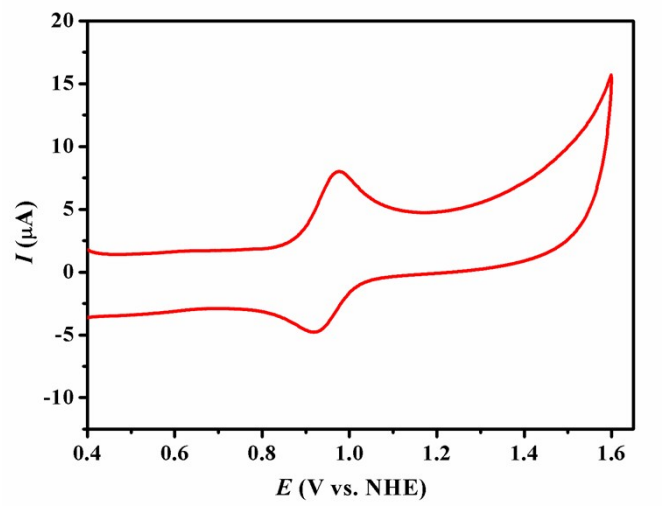

Figure S4. CV curve of **1** in pH 1.0 CF_3SO_3H aqueous solution containing 10% CF_3CH_2OH (scan rate = 100 mV/s).

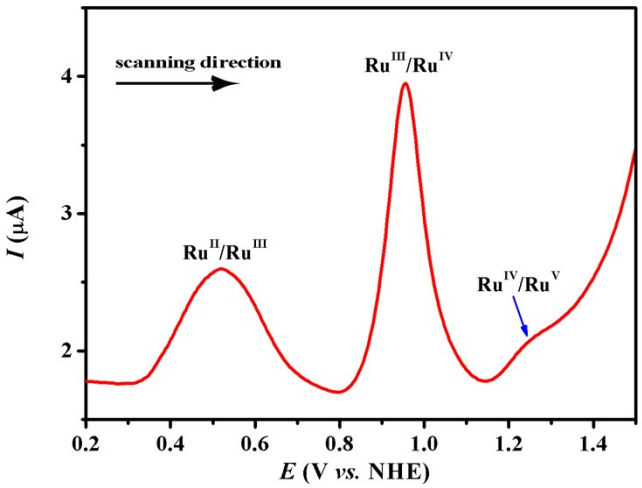

Figure S5. DPV curve of **1** in pH 1.0 CF_3SO_3H aqueous solution containing 10% CF_3CH_2OH.

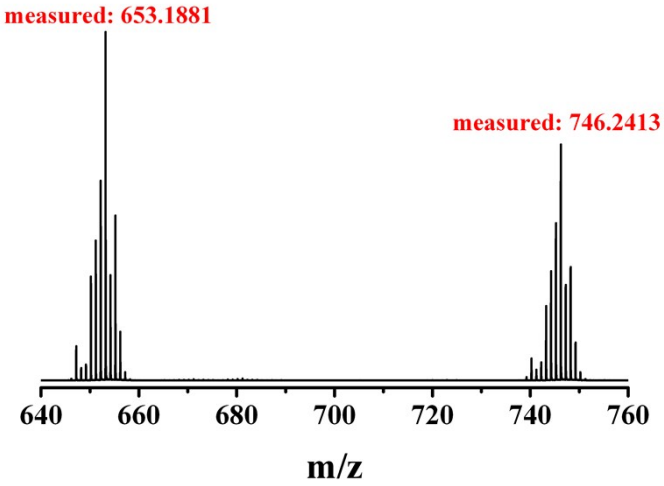

Figure S6. HRMS spectra (positive mode) of $[Ru^{III}(L)(pic)_3 + H]^+$ (calculated: 746.2406) and $[Ru^{III}(L)(pic)_2 + H]^+$ (calculated: 653.1828).

Table S1. Summary of the Metrical Data for **1**.

1	
Empirical formula	C_{40} H_{43} N_4 O_4 Ru, 2(H_2O)
Formula weight	780.89
Crystal system	orthorhombic
Space group	P bca
Temperature/K	298(2)
a/Å	9.758(3)
b/Å	18.451(5)
c/Å	42.443(11)
α/°	90
β/°	90
γ/°	90
V/Å^3	7642(4)
Z	8
Density (calculated)/g cm^{-3}	1.358
Crystal size/mm^3	0.3 × 0.2 × 0.1
F(000)	3256
Theta range for data collection/°	1.92 to 25.01
Absorption coefficient /mm^{-1}	0.461
Reflections collected	32295
Independent reflections	6490 [R_{int} = 0.1737, R_{sigma} = 0.1481]
Index ranges	-11 ≤ h ≤ 8, -21 ≤ k ≤ 21, -50≤ l ≤ 47
Data/restraints/parameters	6490/36/469
Goodness-of-fit on F^2	1.026
Final R indexes [I>=2σ (I)]	R_1 = 0.0785, wR_2 = 0.1434
Final R indexes [all data]	R_1 = 0.1888, wR_2 = 0.1838
Largest diff. peak and hole / e Å^{-3}	0.654/-0.832