Electronic Supplementary Material (ESI) for Dalton Transactions. This journal is © The Royal Society of Chemistry 2019

## **Supporting Information**

Multi-Potential-Step Chronocoulospectrometry for Electrocatalytic Water Oxidation by a Mononuclear Ruthenium Aqua Complex Immobilized on a Mesoporous ITO Electrode

Yuta Tsubonouchi, Junichiro Honta, Taisei Sato, Eman A. Mohamed, Zaki. N. Zahran, Kenji Saito, Tatsuto Yui, Masayuki Yagi\*

Department of Materials Science and Technology, Faculty of Engineering, Niigata University, 8050 Ikarashi-2, Niigata 950-2181, Japan.

## Contents.

## **Calculation of TOF**

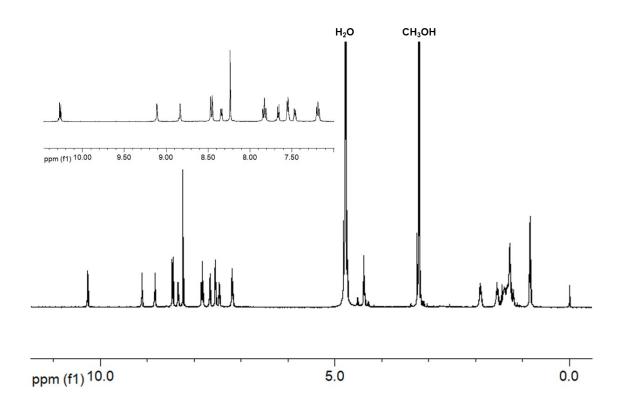
- **Figure S1.**  ${}^{1}\text{H-NMR}$  spectrum of  $[\text{Ru}(\text{C}_{8}\text{Otpy})(\text{H}_{2}\text{dcbpy})\text{Cl}]\text{Cl}$ .
- **Figure S2.** UV-Vis spectrum of  $[Ru(C_8Otpy)(H_2dcbpy)C1]C1$ .
- **Figure S3.**  ${}^{1}\text{H-NMR}$  spectrum of  $[\text{Ru}(\text{C}_{8}\text{Otpy})(\text{H}_{2}\text{dcbpy})(\text{OH}_{2})](\text{NO}_{3})_{2}$ .
- **Figure S4.** UV-Vis spectrum of  $[Ru(C_8Otpy)(H_2dcbpy)(OH_2)](NO_3)_2$ .
- **Figure S5.** XRD patterns of a meso-ITO electrode
- **Figure S6.** FE-SEM images of a meso-ITO electrode.
- **Figure S7.** UV-Vis spectrum of [Ru(C<sub>8</sub>Otpy)(dcbpy)(OH)] in 2 M KOH.

## **Calculation of TOF**

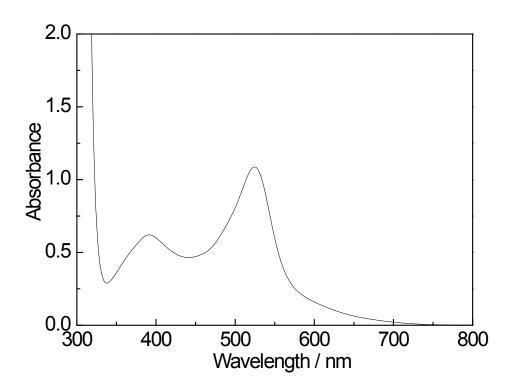
The averaged TOF value during 100 s was calculated from the MPSCCS measurements at the applied potential of 1.5 V vs. Ag/AgCl (Figure 5) according to the following equation:

$$TOF = \frac{Q_{cat} - Q_{blank}}{4 \times F \times \Gamma_{cov} \times t}$$

where,  $Q_{cat}$  [mol/cm<sup>2</sup>] is the charge amount passed during 100 s electrolysis,  $Q_{blank}$  [mol/cm<sup>2</sup>] is the charge amount using an blank meso-ITO electrode,  $\Gamma_{cov}$  [mol/cm<sup>2</sup>] is coverage of **RuOH** on the electrode, F is Faraday constant and t [s] is electrolysis time (100 s).



**Figure S1.** <sup>1</sup>H-NMR spectrum of [Ru(C<sub>8</sub>Otpy)(H<sub>2</sub>dcbpy)Cl]Cl in CD<sub>3</sub>OD.



**Figure S2.** UV-Vis spectrum of [Ru(C<sub>8</sub>Otpy)(H<sub>2</sub>dcbpy)Cl]Cl (0.08 mM) in CH<sub>3</sub>OH.

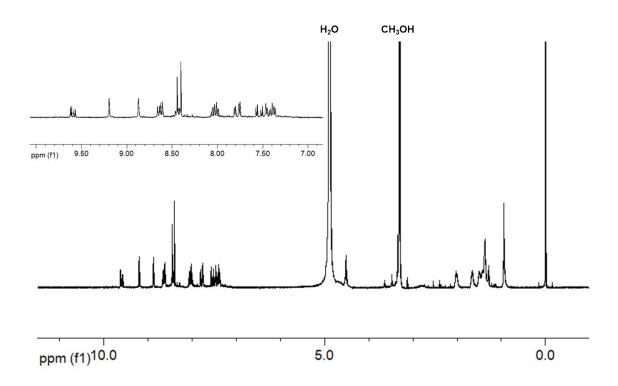
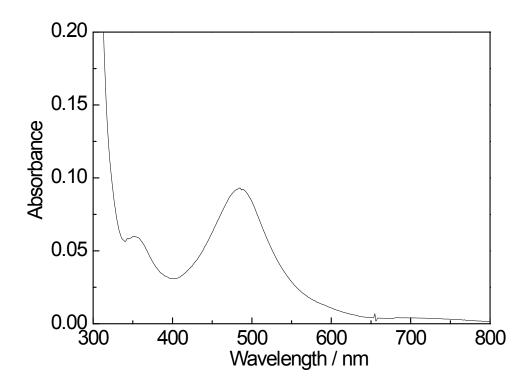
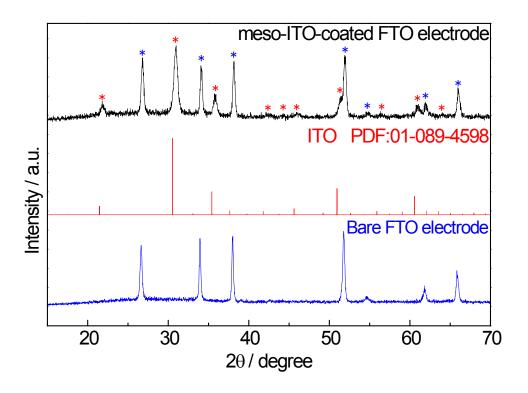


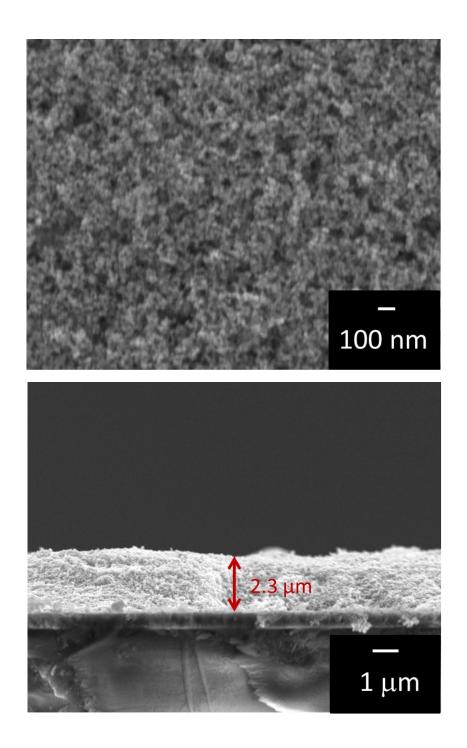
Figure S3.  $^{1}$ H-NMR spectrum of  $[Ru(C_{8}Otpy)(H_{2}dcbpy)(OH_{2})](NO_{3})_{2}$  in  $CD_{3}OD$ .



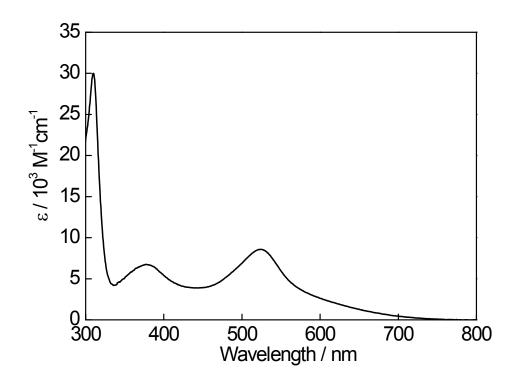
**Figure S4.** UV-Vis spectrum of  $[Ru(C_8Otpy)(H_2dcbpy)(OH_2)](NO_3)_2$  (0.08 mM) in CH<sub>3</sub>OH.



**Figure S5.** XRD patterns of a mesoporous ITO electrode. The peaks for ITO and FTO were marked by the blue and red asterisks, respectively.



**Figure S6.** FE-SEM images of the surface (upper) and cross-section (lower) of a mesoporous ITO electrode.



**Figure S7.** UV-Vis spectrum of  $[Ru(C_8Otpy)(dcbpy)(OH)]^-$  (0.118 mM) in 2 M KOH.