Electronic Supporting Information

Structural Evolution of Ru-bms Complex to The Real Water Oxidation Catalyst of Ru-bda: The Bite Angle Matter

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Table S1. Crystallographic data for **Ru-bms**.

Complex	**Ru-bms**
Empirical formula	$C_{24}H_{29}N_4O_{8.5}RuS_2$
Formula weight	674.70
Temperature/K	296.15
Crystal system	triclinic
Space group	P−1
a/Å	14.085(4)
b/Å	15.200(5)
c/Å	15.861(5)
α/°	109.863(4)
β/°	110.609(4)
γ/°	100.390(4)
Volume/Å^3	2810.3(15)
Z	4
ρ_{calc}g/cm^3	1.595
μ/mm^{-1}	0.762
F(000)	1380.0
Crystal size/mm^3	0.14 × 0.12 × 0.1
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	3.224 to 55.04
Index ranges	-18 ≤ h ≤ 18, -19 ≤ k ≤ 19, -20 ≤ l ≤ 20
Reflections collected	25294
Independent reflections	12640 [R_{int} = 0.0602, R_{sigma} = 0.0984]
Data/restraints/parameters	12640/13/728
Goodness-of-fit on F^2	0.964
Final R indexes [I>=2σ (I)]	R_1 = 0.0506, wR_2 = 0.1072

Final R indexes [all data]	R_1 = 0.0892, wR_2 = 0.1214
Largest diff. peak/hole/e Å^{-3}	0.90/−1.28

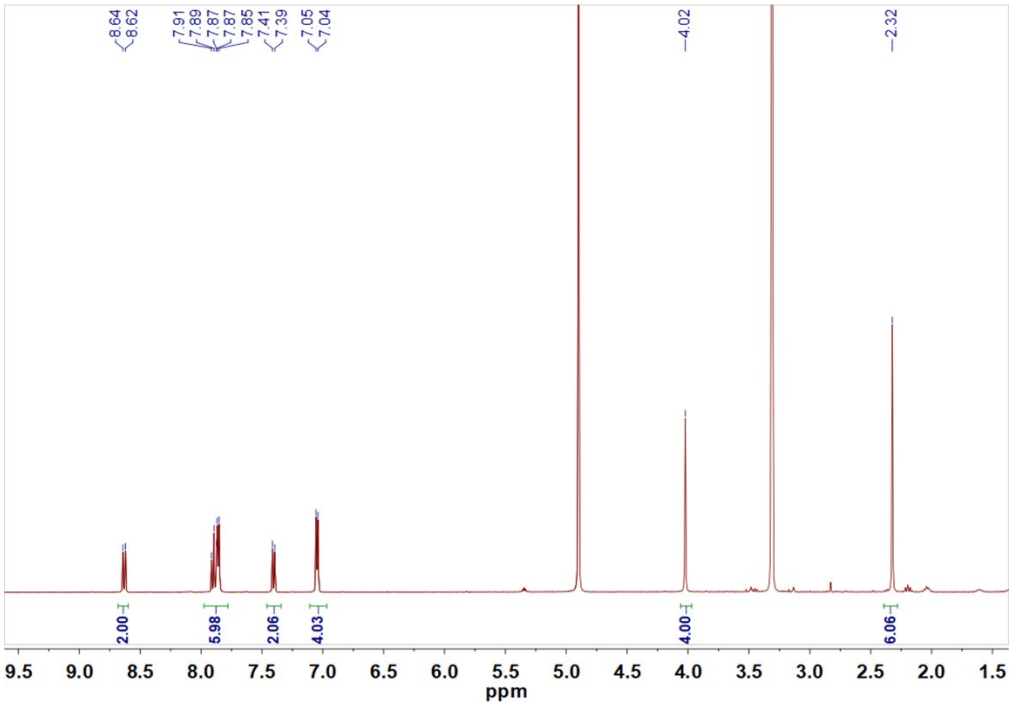

Figure S1. ^{1}H NMR spectrum (400 MHz) of **Ru-bms** in d_4-methanol.

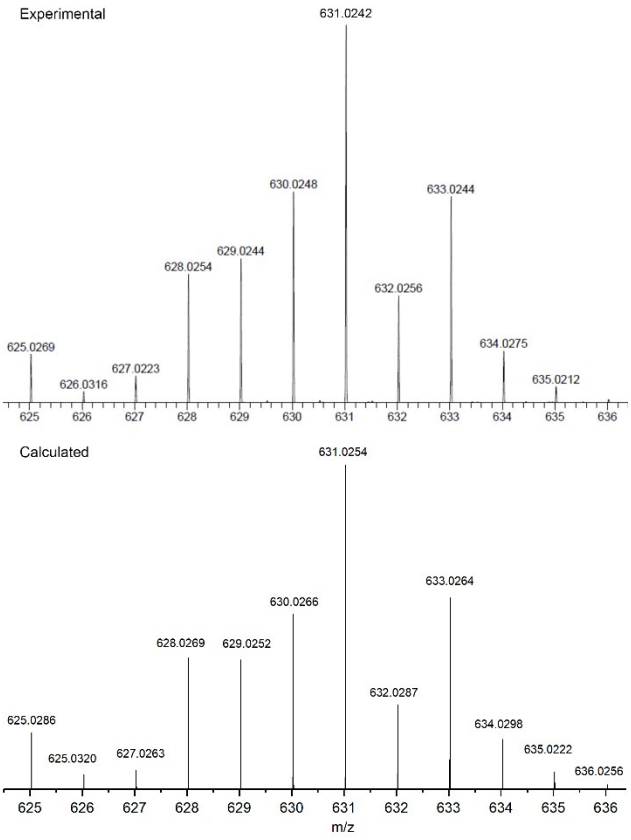

Figure S2. HRMS spectra of [**Ru-bms** + H$^+$] (top) and calculated isotopic distribution (bottom).