Electronic Supplementary Information

Homo-/Heterogeneous Catalysis of Water Oxidation Supported by a Novel Metallamacrocycle

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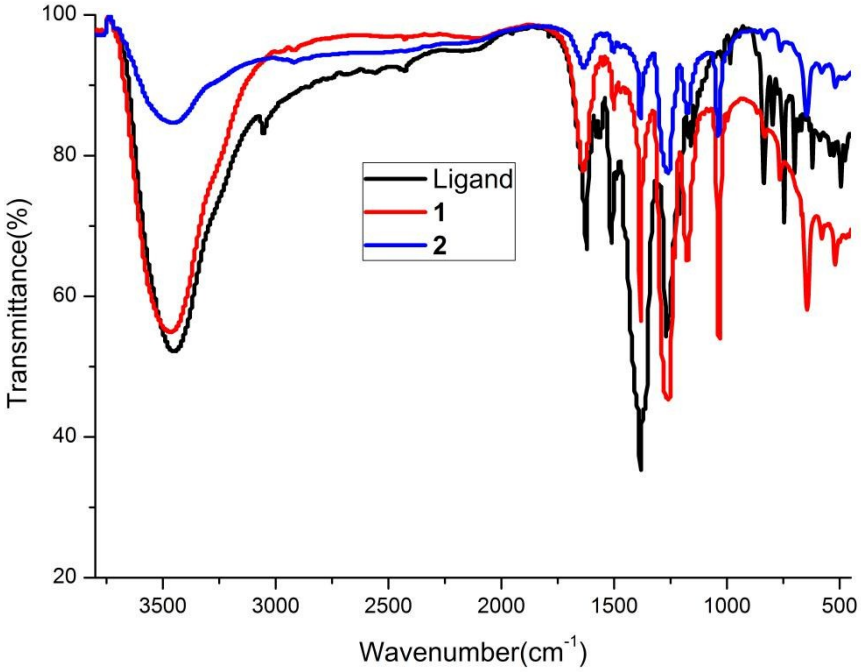

Fig. s1. IR spectra of complexes **1**, **2** and ligand.

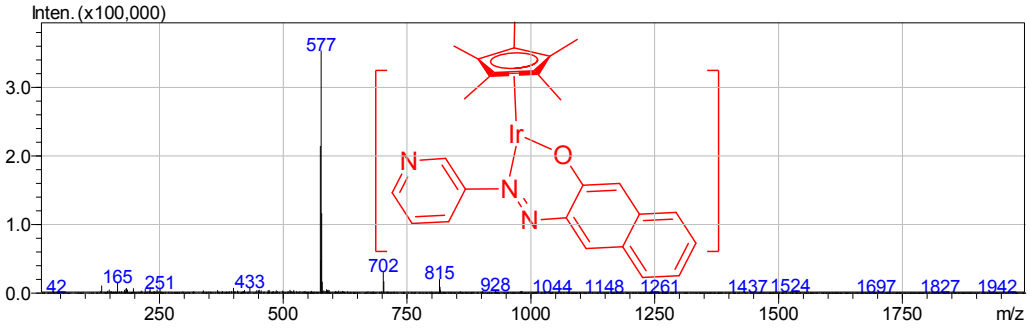

Fig. s2. Ms spectrum of complex **1**.

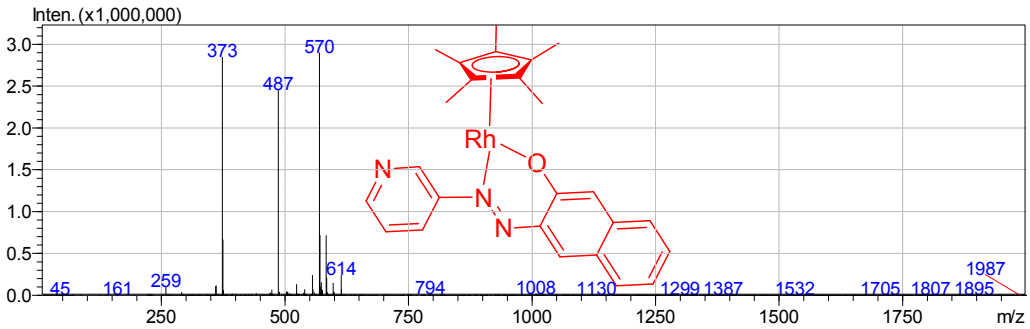

Fig. s3. Ms spectrum of complex **2**.

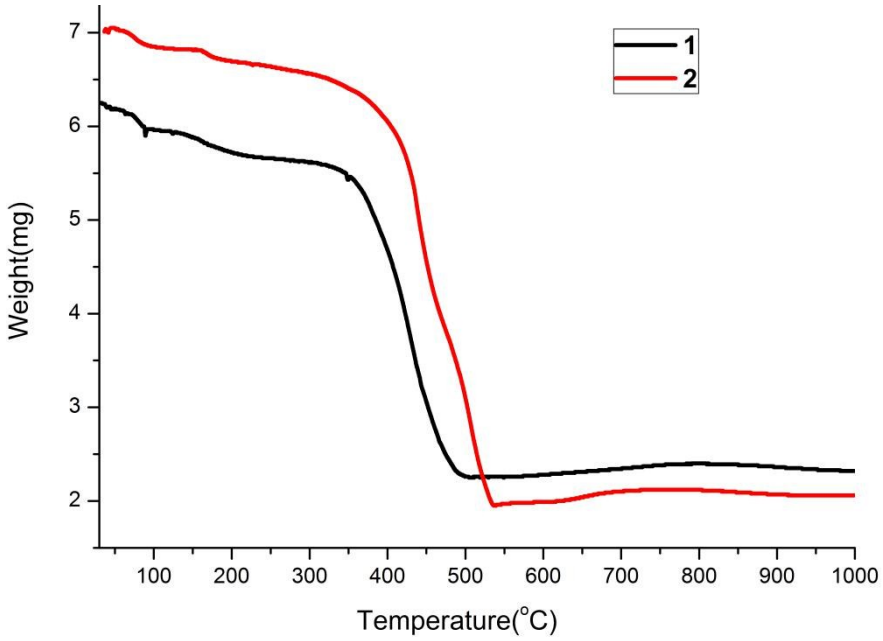

Fig. s4. TGA curves of complex **1** and **2**.

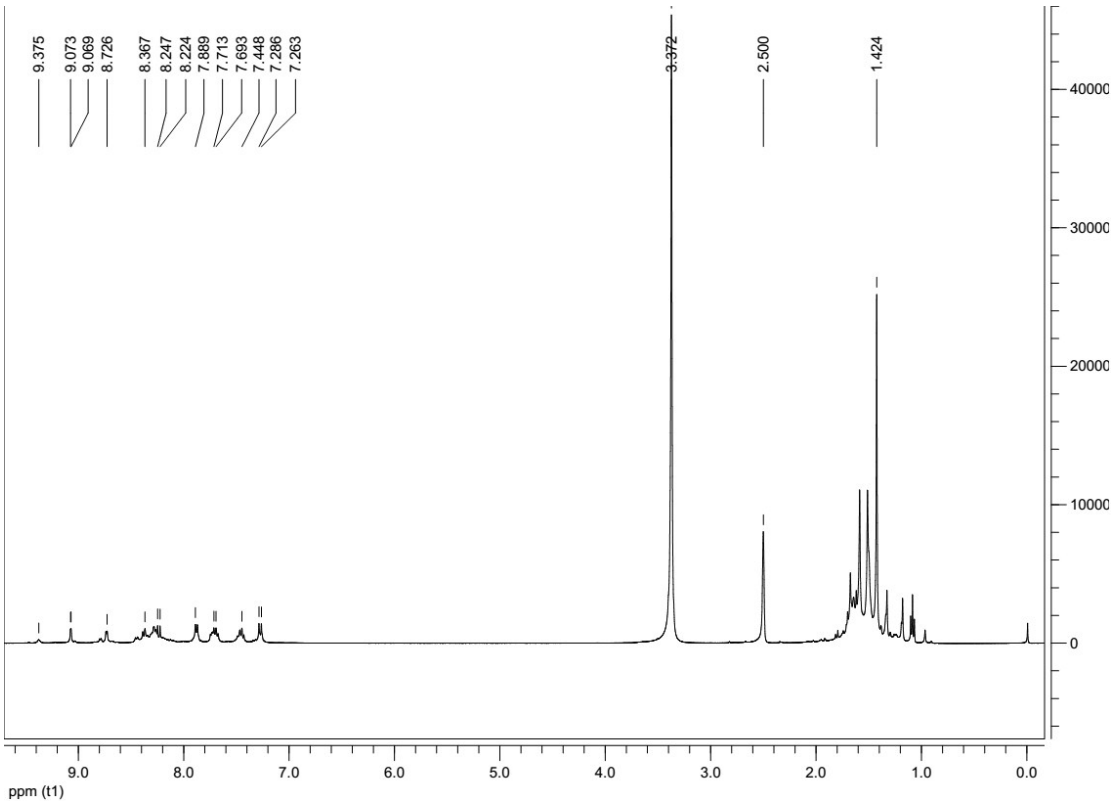

Fig. s5. ^{1}H NMR spectra of **1**.

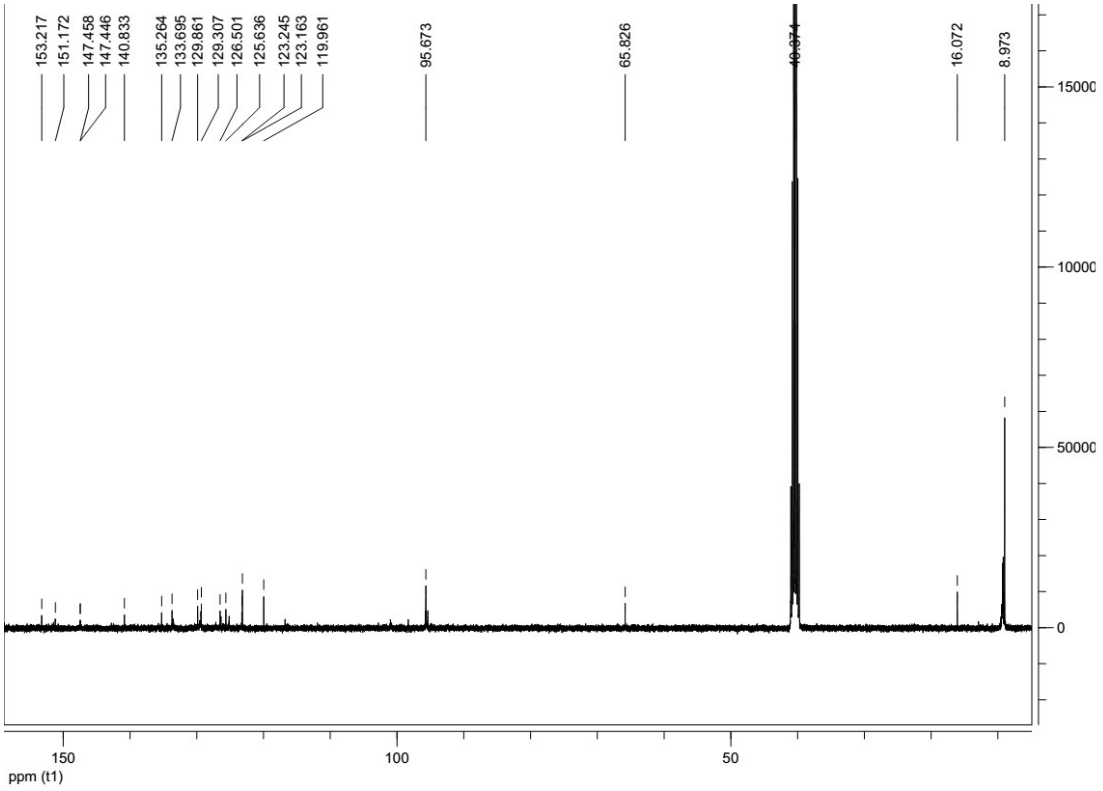

Fig. s6 . ^{13}C NMR of **1**.

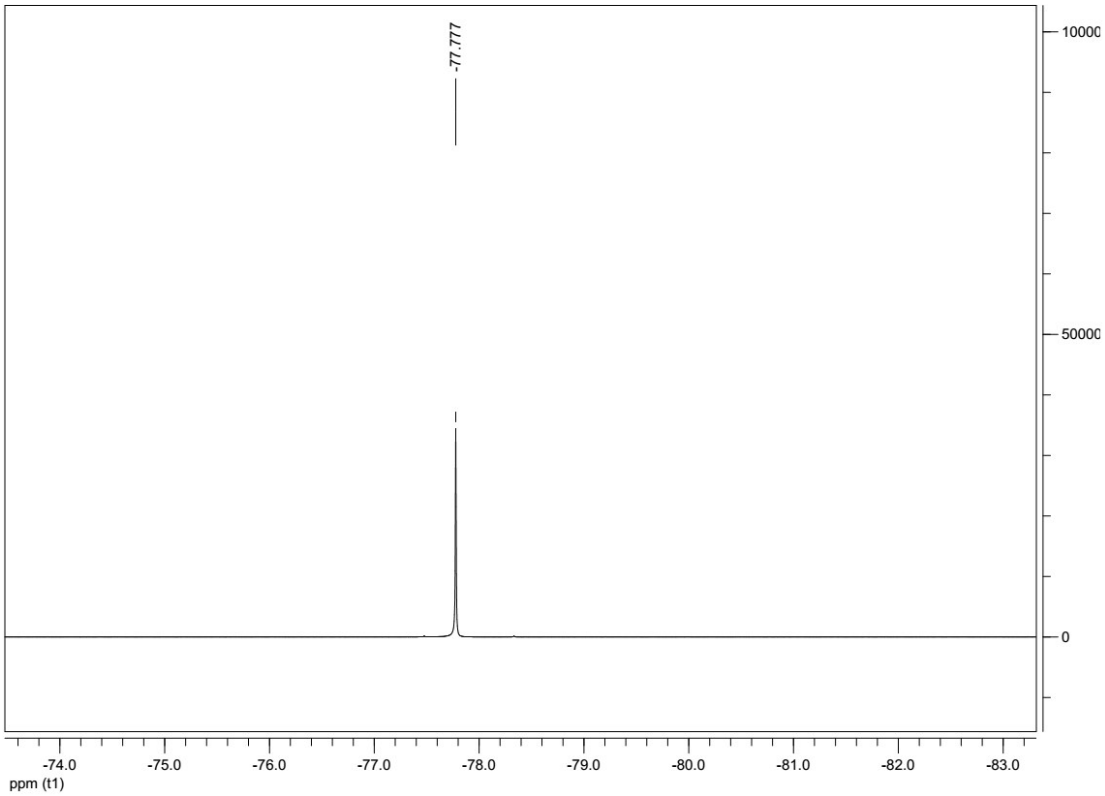

Fig. s7. ^{19}F NMR of **1**

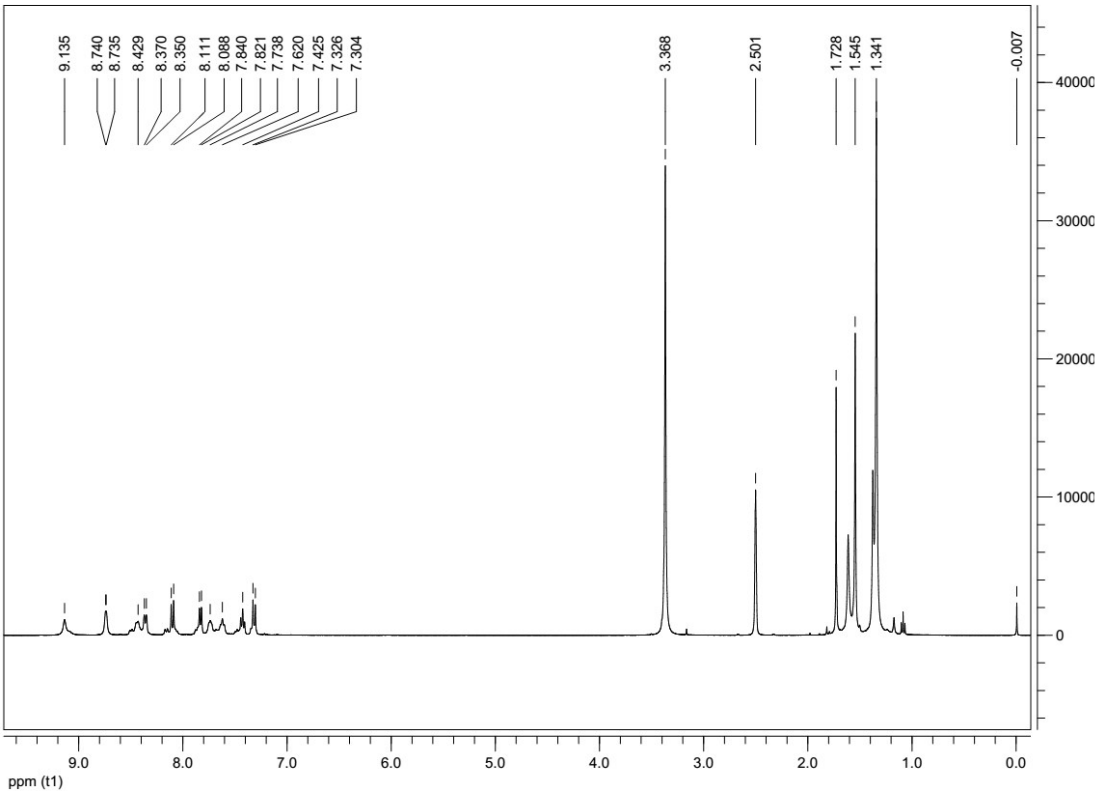

Fig. s8. ^{1}H NMR of **2**.

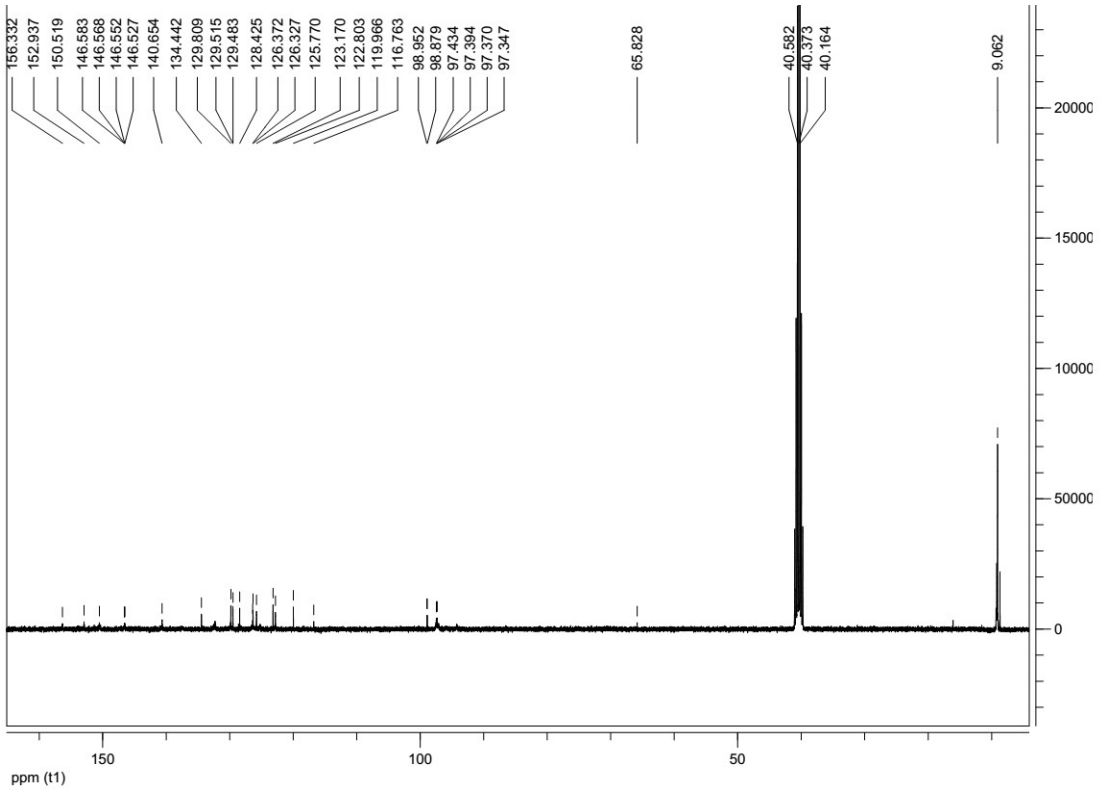

Fig. s9. ^{13}C NMR of **2**.

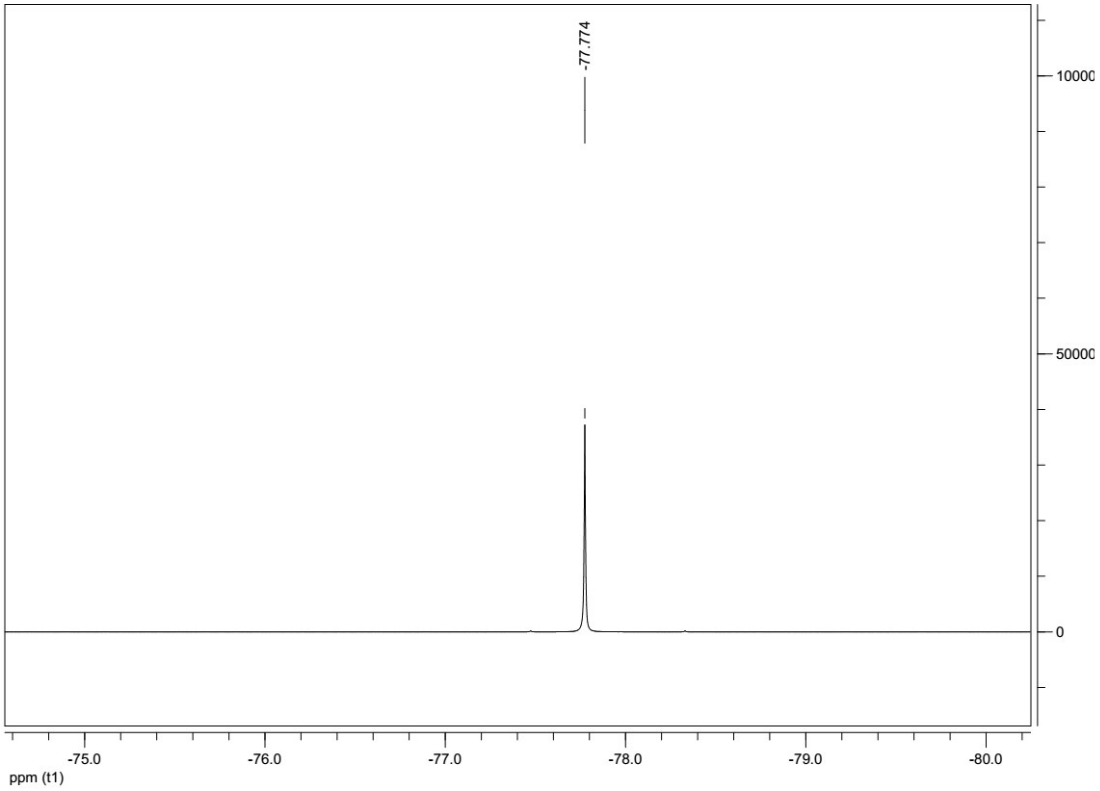

Fig. s10. ^{19}F NMR of **2**.

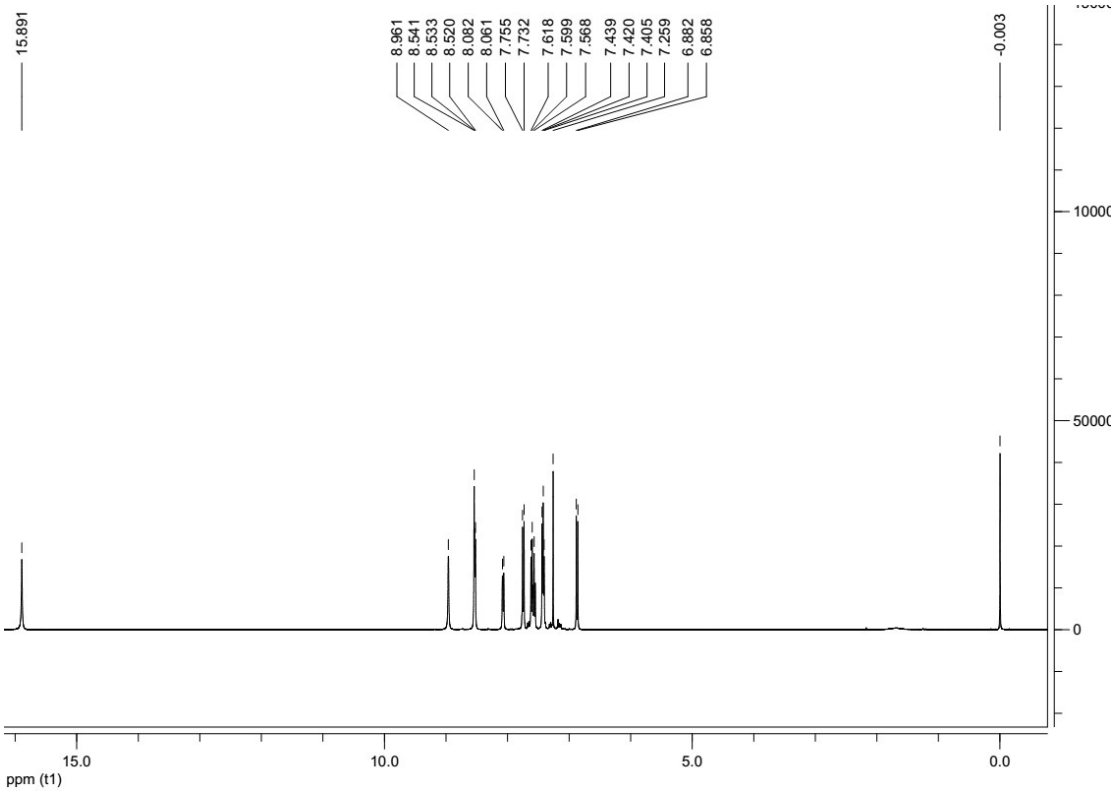

Fig. s11. ^{1}H NMR of ligand.

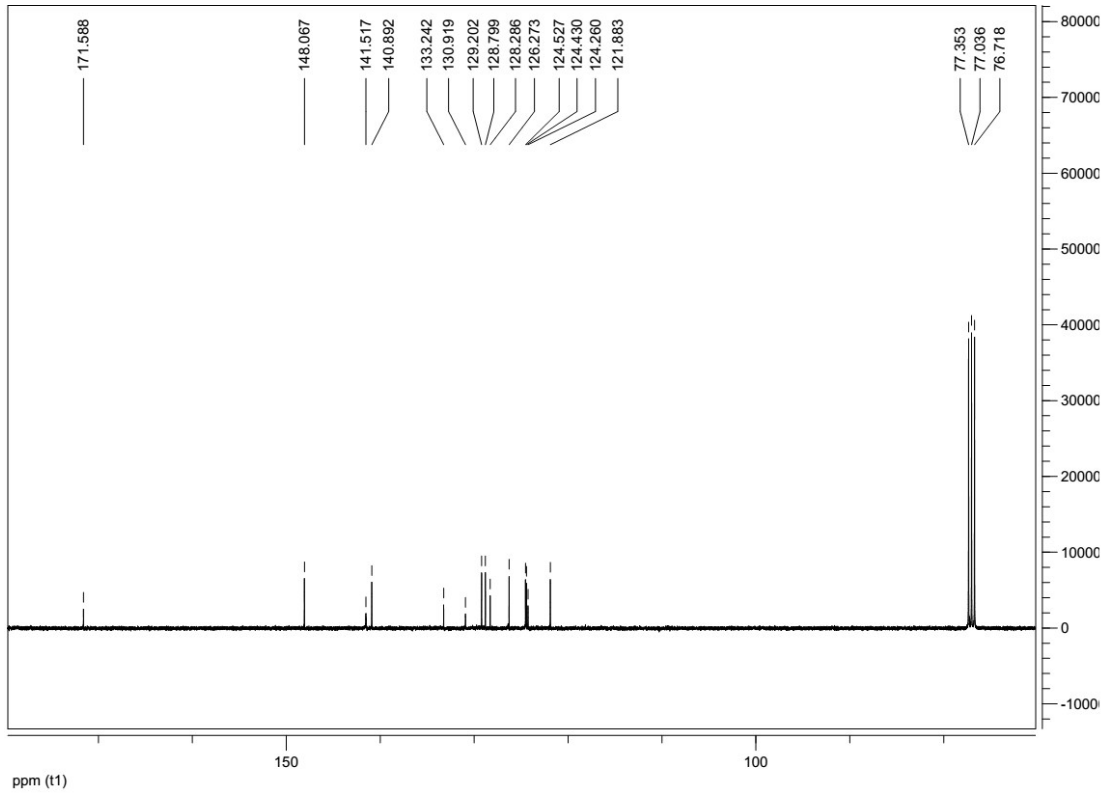

Fig. s12. ^{13}C NMR of ligand.

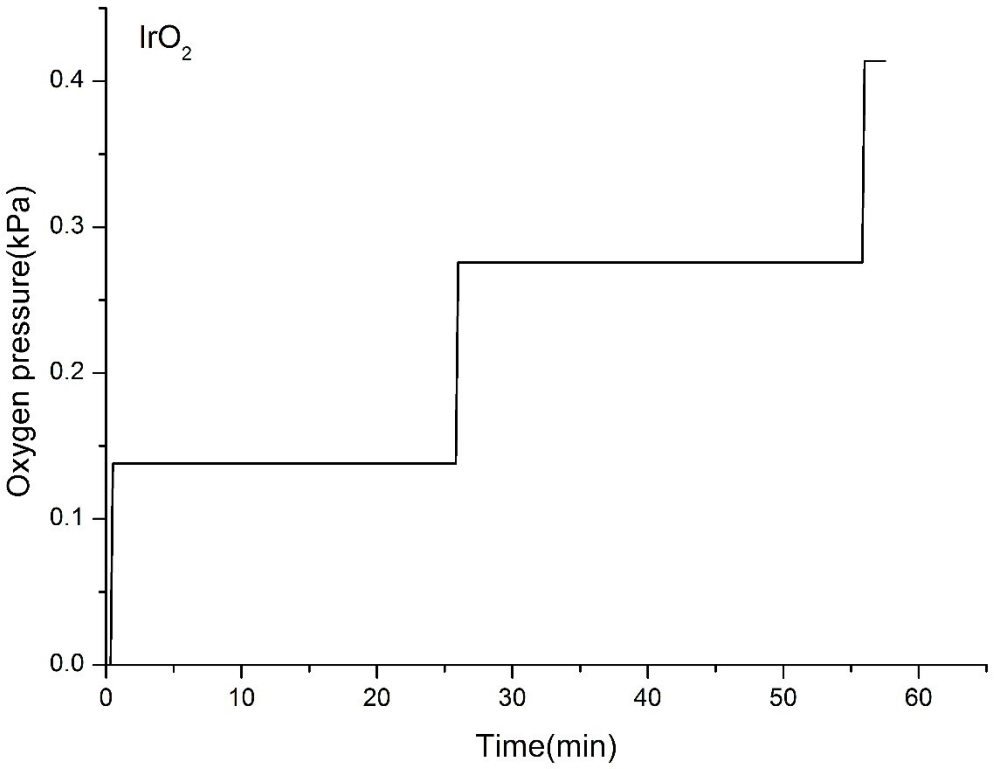

Fig.s12 Oxygen pressure of water oxidation.

Empirical formula	$C_{104}H_{100}F_{12}Ir_4N_{12}O_{16}S_4$
Formula weight	2899.00
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 14.964(8) A alpha = 90 deg. b = 24.495(14) A beta = 109.982(6) deg. c = 15.987(9) A gamma = 90 deg.
Volume	5507(5) A^3
Z, Calculated density	2, 1.748 Mg/m^3
Absorption coefficient	4.981 mm^-1
F(000)	2832
Crystal size	0.25 x 0.22 x 0.20 mm
Theta range for data collection	2.21 to 27.40 deg.
Limiting indices	-16<=h<=19, -19<=k<=31, -20<=l<=20

Reflections collected / unique	31830 / 12186 [R(int) = 0.1263]
Completeness to theta = 27.71	97.3 %
Max. and min. transmission	0.4357 and 0.3690
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12186 / 732 / 680
Goodness-of-fit on F^2	0.949
Final R indices [I>2sigma(I)]	R1 = 0.0907, wR2 = 0.2306
R indices (all data)	R1 = 0.1856, wR2 = 0.2917
Largest diff. peak and hole	3.591 and -2.681 e.A^-3

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

Empirical formula	$C_{52}H_{50}F_6N_6O_8Rh_2S_2$
Formula weight	1270.92
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 14.940(4) A alpha = 90 deg. b = 24.403(6) A beta = 109.611(3) deg. c = 15.917(4) A gamma = 90 deg.
Volume	5467(2) A^3
Z, Calculated density	4, 1.544 Mg/m^3
Absorption coefficient	0.758 mm^-1
F(000)	2576
Crystal size	0.22 x 0.18 x 0.15 mm
Theta range for data collection	2.15 to 27.68 deg.
Limiting indices	-19<=h<=19, -31<=k<=30, -19<=l<=20
Reflections collected / unique	33536 / 12591 [R(int) = 0.0606]
Completeness to theta = 27.71	98.5 %
Max. and min. transmission	0.8948 and 0.8510
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12591 / 731 / 695
Goodness-of-fit on F^2	1.096
Final R indices [I>2sigma(I)]	R1 = 0.0721, wR2 = 0.1872
R indices (all data)	R1 = 0.1206, wR2 = 0.2075
Largest diff. peak and hole	1.647 and -1.099 e.A^-3

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