Supplementary Information

For

Re(VII) complex of N-fused tetraphenylporphyrin

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1. Experimental Section

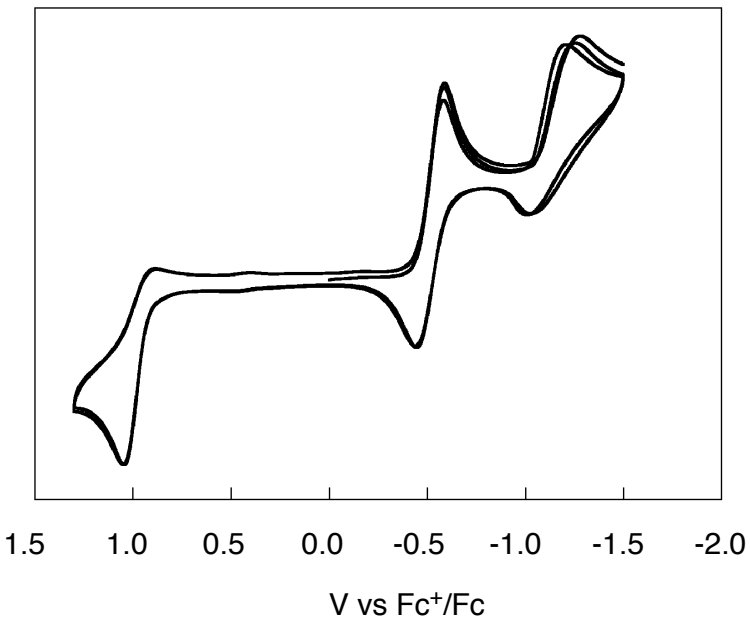
Synthesis of $NFpReO_3$ (2)

A suspension of $NFpRe(CO)_3$ (**1**, 30 mg, 34 μmol, 1.0 equiv) and $Me_3NO \cdot 2H_2O$ (30 mg, 0.27 mmol, 7.9 equiv) in 1,2-dichlorobenzene (15 ml) was heated at 140 °C for 30 min. After cooling, 1,2-dichlorobenzene was removed under reduced pressure and the residue was purified by silica gel column chromatography (eluent: CH_2Cl_2). The first violet fraction gave recovered **1** and the second violet fraction gave **2** in 32% yield (9.1 mg, 11 μmol). IR (powder, cm^{-1}): 932.0, 907.7 (Re=O); ^1H NMR ($CDCl_3$, 300 MHz, ppm): δ 7.43 (d, J = 4.3 Hz, 1H), 7.57–7.66 (m, 5H), 7.66–7.85 (m, 9H), 7.86-7.92 (m, 2H), 7.97 (d, J = 4.9 Hz, 1H), 8.02-8.08 (m, 2H), 8.21-8.26 (m, 2H), 8.72 (d, J = 7.3 Hz, 2H), 8.91 (d, J = 4.9 Hz, 1H), 9.37 (d, J = 4.9 Hz, 1H), 9.38 (s, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz, ppm): δ 112.11, 113.01, 120.66, 121.95, 124.33, 126.31, 127.47, 127.70, 128.09, 128.34, 128.64, 128.74, 128.84, 129.65, 129.69, 129.96, 130.05, 132.65, 132.77, 133.27, 134.25, 134.52, 136.83, 137.09, 137.63, 137.97, 139.36, 142.75, 144.75, 150.29, 154.20, 154.68, 155.41, 159.91, 162.56; MS (MALDI, positive): 812 ($[M–2O]^+$), 828 ($[M–O]^+$), 844 ($[M]^+$); UV-vis (CH_2Cl_2, λ_{max}/nm (ε)): 375 (47000), 442 (26000), 520 (60000), 994 (3600); R_f = 0.33 (silica gel 60, eluent: CH_2Cl_2).

Oxygen transfer reaction catalyzed by 2

Triphenylphosphine (306 mg, 1.17 mmol) was added to a solution of 4-phenylpyridine *N*-oxide (200 mg, 1.17 mmol) and **2** (9.80 mg, 1mol%) in toluene. The resulting solution was stirred at 26 °C for 1 h. After removal of the solvent under reduced pressure, the residue was purified by silica gel column chromatography with CH_2Cl_2 to give 4-phenylpyridine in 99% yield (180 mg, 1.16 mmol).

2. CV data of 2



Cyclic voltammogram of **2** (multiple scan between –1.95 V and +0.86 V): 0.1 M Bu_4NPF_6 in CH_2Cl_2 at 24 °C with a Pt working electrode. Scan rate = 100 mV/s.