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**SUPPORTING INFORMATION**

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**Title:** Mono- and Dinuclear Complexes of Tricarbonylrhenium(I) with 4-Methyl-2,2'-bipyridine-4'-carbonitrile

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Table S1. Crystallographic data for complex **2**.

empirical formula	C <sub>24</sub> H <sub>20</sub> F <sub>6</sub> N <sub>4</sub> O <sub>3</sub> Pre
Formula weight	743.61
Crystal system	Triclinic
Space Group	P-1
a[Å]	10.3311(10)
b[Å]	10.5109(10)
c[Å]	13.3382(12)
α [°]	71.804(2)
β [°]	84.398(2)
γ [°]	76.811(2)
V [Å <sup>3</sup> ]	1339.1(2)
Formula Units/ cell	2
Temp,K	293.2
ρ <sub>calc</sub> , [Mg/m <sup>-3</sup> ]	1.844
μ[mm <sup>-1</sup> ]	0.626
Final R indices, [I>2σ(I)]	R <sub>1</sub> =0.0269; wR <sub>2</sub> = 0.0623
R indices [all data]	R <sub>1</sub> =0.0304; wR <sub>2</sub> = 0.0644

$$R_1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}; wR_2 = \frac{[\sum \{w(F_o^2 - F_c^2)^2\} / \sum \{w(F_o^2)^2\}]^{1/2}}{\sum \{w(F_o^2)^2\}^{1/2}}$$

where  $w = 1/[\sigma^2(F_o^2) + (0.0042P)^2]$  and  $P = (F_o^2 + 2F_c^2)$

Table S2. Selected bond lengths [Å] and angles [°] for complex **2**.

Re(1)-C(15)	1.915(3)
Re(1)-C(17)	1.915(3)
Re(1)-C(16)	1.925(4)
Re(1)-N(4)	2.138(3)
Re(1)-N(1)	2.162(3)
Re(1)-N(2)	2.173(3)
C(11)-N(3)	1.140(5)
C(15)-Re(1)-C(17)	89.25(14)
C(15)-Re(1)-C(16)	89.39(15)
C(17)-Re(1)-C(16)	88.78(14)
C(15)-Re(1)-N(4)	177.83(11)
C(17)-Re(1)-N(4)	90.86(13)
C(16)-Re(1)-N(4)	92.77(13)
C(15)-Re(1)-N(1)	92.79(12)
C(17)-Re(1)-N(1)	98.03(12)
C(16)-Re(1)-N(1)	172.87(11)
N(1)-Re(1)-N(2)	74.51(10)

Table S3. Emission spectral fitting results.

Complex	$E_0(\text{cm}^{-1})^{[a]}$	$h\nu_M(\text{cm}^{-1})^{[a]}$	$S_M^{[a]}$	$\Delta\nu_{0,1/2}(\text{cm}^{-1})^{[a]}$	$E_0(\text{cm}^{-1})^{[b]}$	$\Delta\nu_{0,1/2}(\text{cm}^{-1})^{[b]}$
<b>1</b>	$17439 \pm 21$	$1406 \pm 12$	$0,85 \pm 0,026$	$2623 \pm 47$	$14560 \pm 16$	$3231 \pm 44$
<b>2</b>	$19540 \pm 05$	$1520 \pm 04$	$0,76 \pm 0,006$	$2284 \pm 11$	$16588 \pm 05$	$2838 \pm 15$
<b>3</b>	$21465 \pm 11$	$1368 \pm 10$	$0,60 \pm 0,014$	$3080 \pm 42$	$17010 \pm 07$	$3492 \pm 23$
<b>4</b>	$18775 \pm 20$	$1542 \pm 08$	$0,47 \pm 0,024$	$2970 \pm 53$	$17270 \pm 08$	$3776 \pm 28$

<sup>[a]</sup> 77 K in 4:1 (v:v) Ethanol-Methanol . <sup>[b]</sup> r.t. in CH<sub>3</sub>CN.

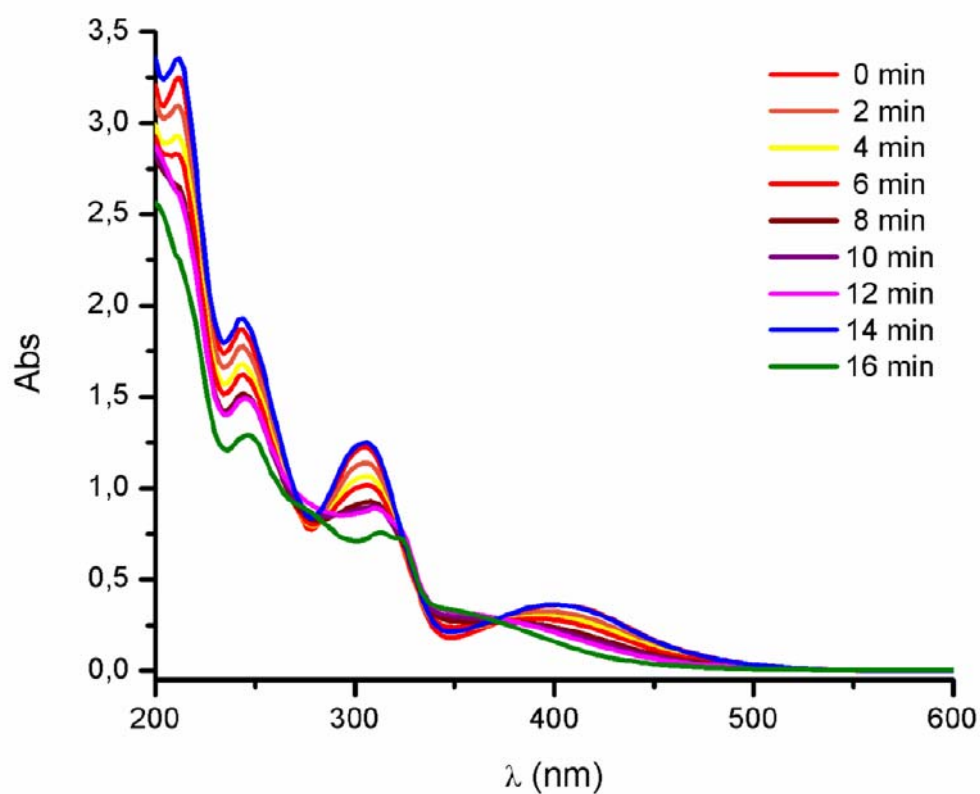


Fig. S1. Controlled potential electrolysis at  $V = -1.0$  V of  $[\text{Re}(\text{Meppy-CN})(\text{CO})_3\text{Cl}]$  (complex **1**) to give  $[\text{Re}(\text{Meppy-C}(\text{O})\text{NH}_2)(\text{CO})_3(\text{CH}_3\text{CN})]^+$ .

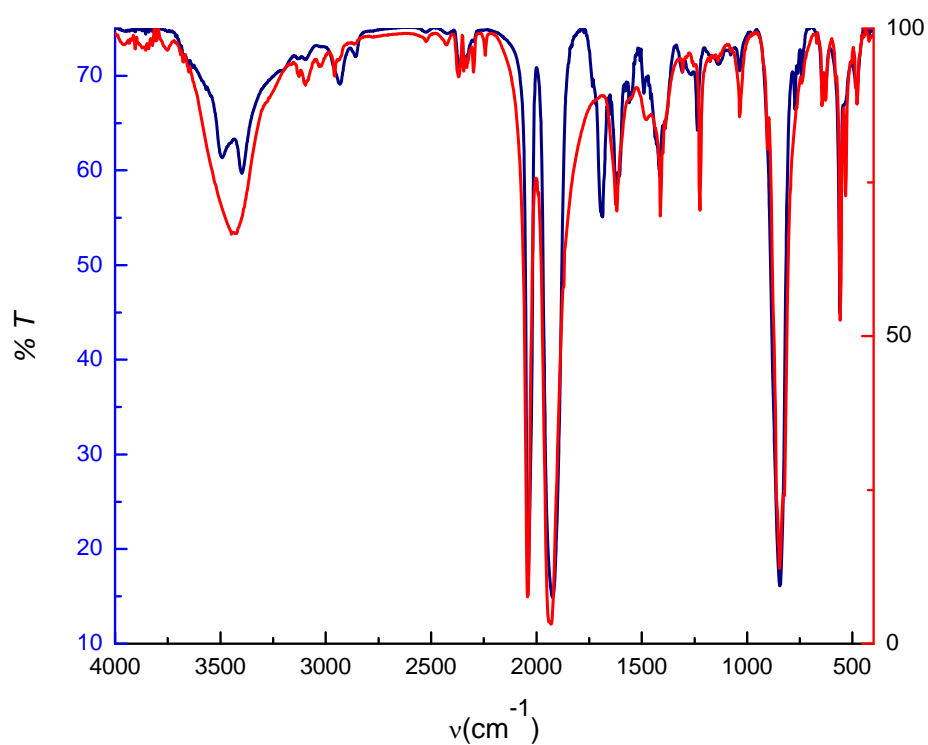


Fig. S2. IR spectra as KBr pellets of: 1-  $[\text{Re}(\text{Mebpy-CN})(\text{CO})_3\text{Cl}]$  (red line) and 2-  $[\text{Re}(\text{Mebpy-C}(\text{O})\text{NH}_2)(\text{CO})_3(\text{CH}_3\text{CN})]^\dagger$  (blue line).

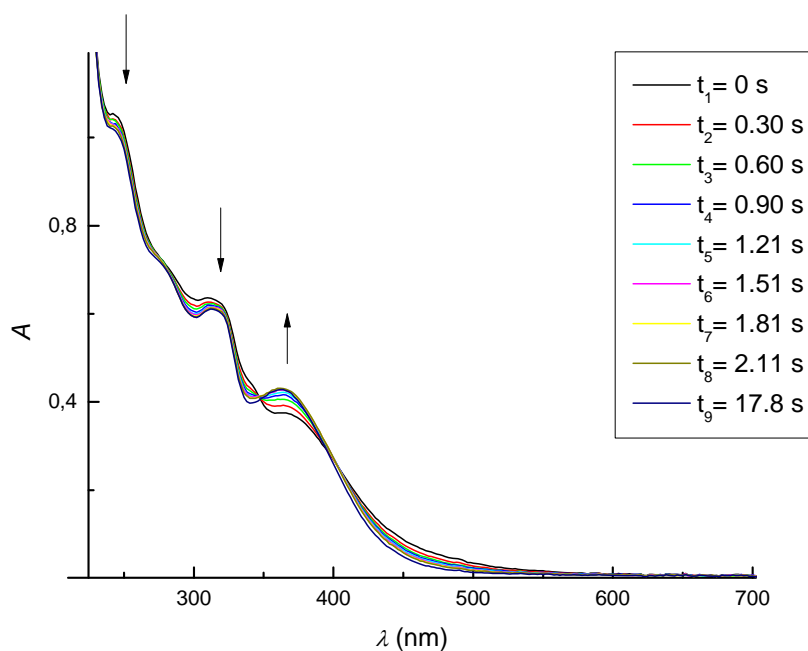


Fig. S3. Consecutive UV/Vis spectra obtained when dissolving aqueous solutions of complex **3** ( $C = 2.4 \times 10^{-4}$  M) and  $\text{K}_2\text{S}_2\text{O}_8$  ( $C = 2.4 \times 10^{-3}$  M) at r.t., pH = 3.0 ( $\text{CF}_3\text{COOH}$ ),  $I = 0.1$  M (KCl).