Mono- and di-nuclear Re(I) complexes and the role of protonable nitrogen atom on quenching emission process by hydroquinone

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Supplementary Information



Figure S1: ¹H NMR spectrum of fac-[Re(CO)₃(ph₂phen)(4,4'-bpy)]⁺ in CD₃CN at 25°C (300MHz).



Figure S2: ¹H NMR spectrum of $[{(ph_2phen)(CO)_3Re}_2(4,4'-bpy)]^{2+}$ in CD₃CN at 25°C (500MHz).

Compound	Proton	δ (ppm)	J (Hz)
$ \begin{array}{c} a^{a} \\ b^{b} \\ a^{c} \\ c^{c} $	$\begin{array}{l} H_{\alpha} \\ H_{\beta} \\ H_{\delta} \\ H_{\gamma} \\ H_{a} \\ H_{a'} \\ H_{b} \\ H_{b'} \end{array}$	9.67 (d,2H) 8.07 (d, 2H) 8.09 (s, 2H) 7.65 (m, 10H) 8.65 (dd, 2H) 8.46 (dd, 2H) 7.55 (dd, 2H) 7.50 (dd, 2H)	5.4 5.4 4.5; 1.8 5.2; 1.7 4.5; 1.5 5.1; 1.5
$ \begin{array}{c} & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & $	$\begin{array}{l} H_{\alpha} \\ H_{\beta} \\ H_{\delta} \\ H_{\gamma} \\ H_{a} \\ H_{b} \end{array}$	9.61 (d, 4H) 8.04 (d, 4H) 8.06 (s, 4H) 7.64-7.59 (m, 20H) 8.40 (dd, 4H) 7.36 (dd, 4H)	5.5 5.2 5.5; 1.5 5.2; 1.5

Table S1. ¹H NMR spectral data for rhenium(I) complexes in CD₃CN (300 or 500 MHz).



Figure S3: FTIR spectra of *fac*-[Re(CO)₃(ph₂phen)(4,4'-bpy)]PF₆ (—) and [{(ph₂phen)(CO)₃Re}₂(4,4'-bpy)](PF₆)₂ (—).



Figure S4: Differential pulse voltammogram of fac-[Re(CO)₃(ph₂phen)(4,4'-bpy)]⁺ in acetonitrile solution (0.1 M LiClO₄).



Figure S5: Differential pulse voltammogram of $[{(ph_2phen)(CO)_3Re}_2(4,4'-bpy)]^{2+}$ in acetonitrile solution (0.1 M LiClO₄).



Figure S6: Cyclic voltammogram of mono-nuclear *fac*-[Re(CO)₃(ph₂phen)(4,4'-bpy)]⁺ (-) and of di-nuclear [{(ph₂phen)(CO)₃Re}₂(4,4'-bpy)]⁺² (-) in acetonitrile solution (0.1 M LiClO₄) and scan rate: 100 mV.s⁻¹.



Figure S7. Emission spectra of mononuclear *fac*-[Re(CO)₃(ph₂phen)(4,4'-bpy)]⁺ (A) and of dinuclear [$\{(ph_2phen)(CO)_3Re\}_2(4,4'-bpy)$]⁺² (B) complexes in CH₃CN at 298 K.



Figure S8: Emission spectra, luminescence decay and Stern-Volmer plots of $[{(p_2phen)(CO)_3Re}_2(4,4'-bpy)]^{2+}$ in CH₃CN in the presence of different concentrations of hydroquinone at 298 K.



Figure S9: Absorption spectra of *fac*-[Re(CO)₃(ph₂phen)(4,4'-bpy)]⁺ in CH₃CN in the presence of different concentrations of hydroquinone at 298 K. Inset: Absorption spectra of hydroquinone in CH₃CN at 298 K in three different concentration.



Figure S10: Absorption spectra of $[{(ph_2phen)(CO)_3Re}_2(4,4^2-bpy)]^{2+}$ in CH₃CN in the presence of different concentrations of hydroquinone at 298 K. Inset: Absorption spectra of hydroquinone in CH₃CN at 298 K in three different concentration.