

Photophysical properties of rhenium(I) complexes and photosensitized generation of singlet oxygen

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Electronic Supporting Information

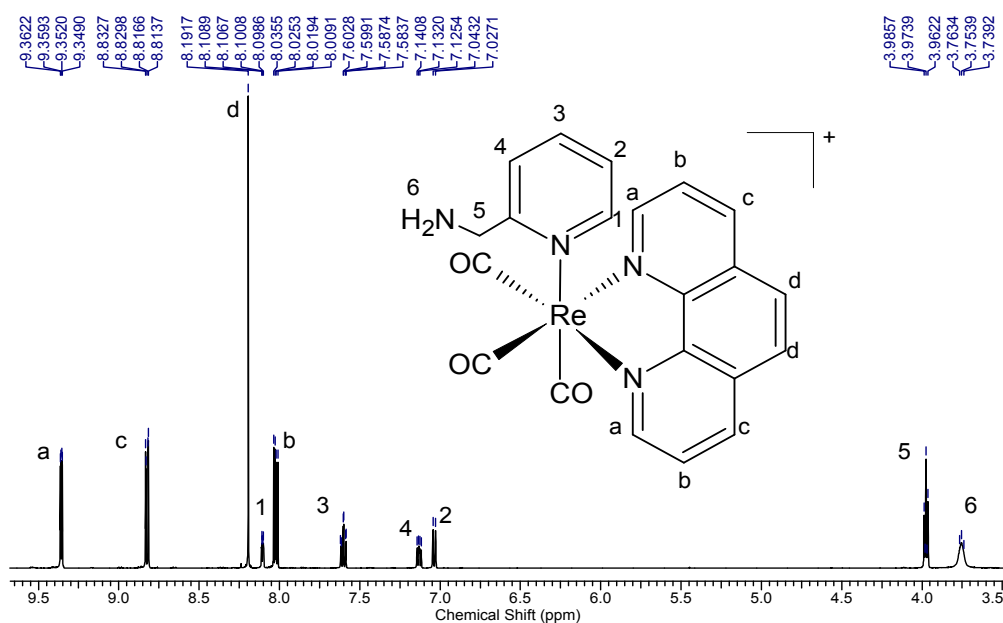


Figure 1S: ^1H NMR spectrum of $\text{fac-}[\text{Re}(\text{CO})_3(\text{phen})(\text{ampy})]^+$ in CD_3CN at 25°C (500MHz).

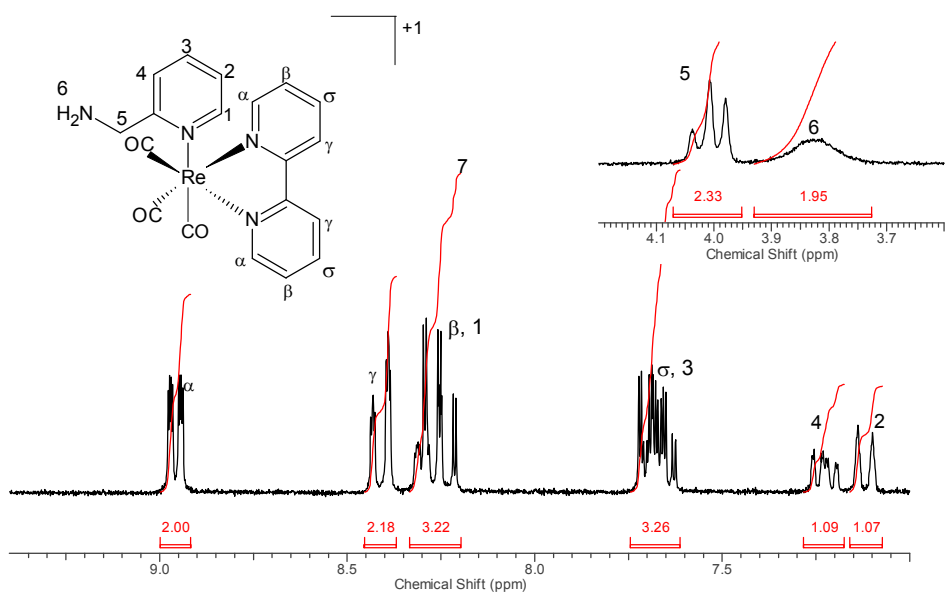
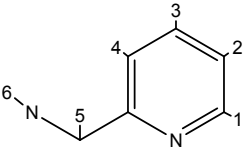
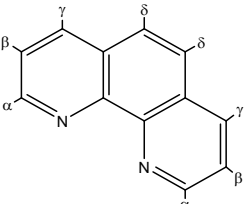
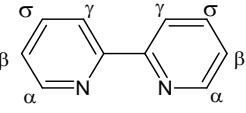
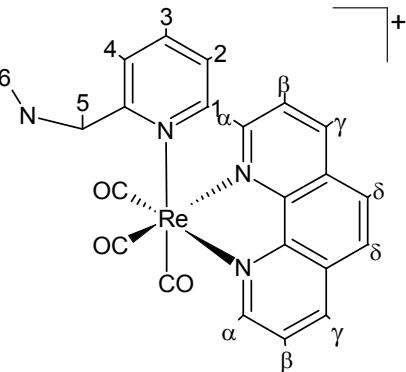
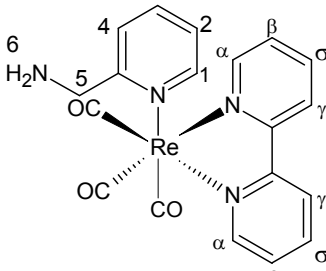


Figure 2S: ^1H NMR spectrum of $\text{fac-}[\text{Re}(\text{CO})_3(\text{bpy})(\text{ampy})]^+$ in CD_3CN at 25°C (200MHz).

Table 1S: ¹H NMR spectral data for rhenium(I) complexes and ligands.

Compound	Proton	δ (ppm)	J (Hz)	ref
	H1 H2 H3 H4 H5 H6	8.3 7.2 7.8 7.3 3.7		1
	H α H β H γ H δ	9.14 7.52 8.10 7.62		2
	H α (d) H γ (d) H β (t) H σ (t)	8.65 8.40 7.23 7.74		
	H α (dd) H β (dd) H γ (dd) H δ (s) H1 (dd) H2 (dd) H3 (td) H4 (d) H5 (t) H6 (band)	9.35 8.02 8.82 8.25 8.10 7.13 7.60 7.03 3.97 3.75	5.0; 1.5 8.2; 5.0 8.2; 1.5 5.0; 1.5 5.0; 7.5 7.5; 2.0 7.5 6.0	
	H α (d) H γ (d) H β ,1 (m) H σ ,H3 (m) H2 (t) H4 (d) H5 (t) H6 (band)	8.95 8.41 8.27 7.68 7.13 7.48 4.01 3.83	5.5 8.3 1.2; 6.7 7.8 5.8 -	

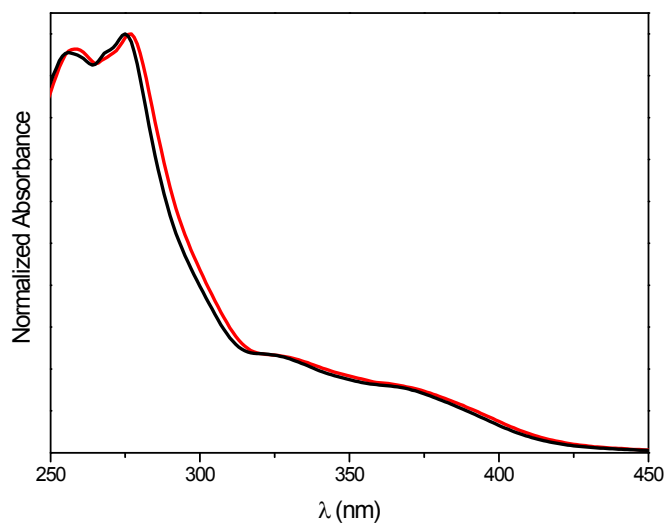


Figure 3S. UV-Vis spectra of $fac-[Re(ampy)(CO)_3(phen)]^+$ in CH_3CN (—) and in PMMA (—) at 25 °C.

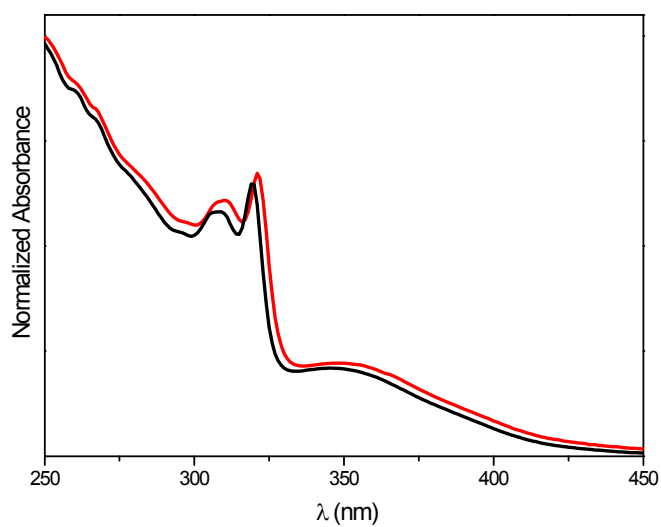


Figure 4S. UV-Vis spectra of $fac-[Re(ampy)(CO)_3(bpy)]^+$ in CH_3CN (—) and in PMMA (—) at 25 °C.

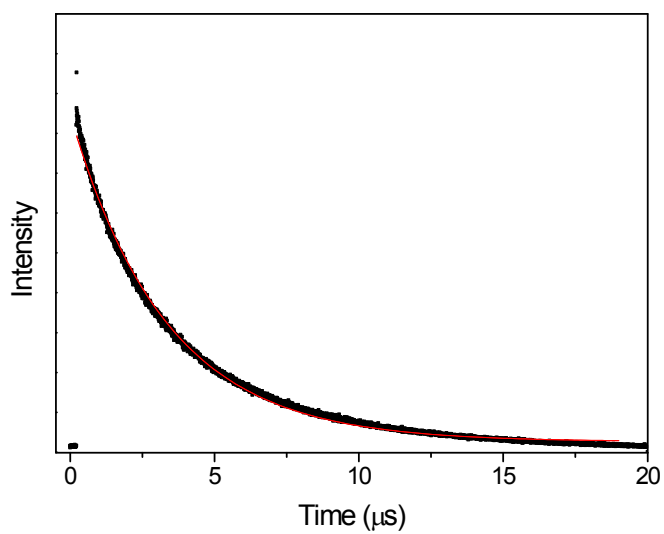


Figure 5S: Time-resolved decay curves of $fac-[Re(ampy)(CO)_3(phen)]^+$ (probed at maxima wavelength after 375 nm laser excitation in PMMA at 298 K).

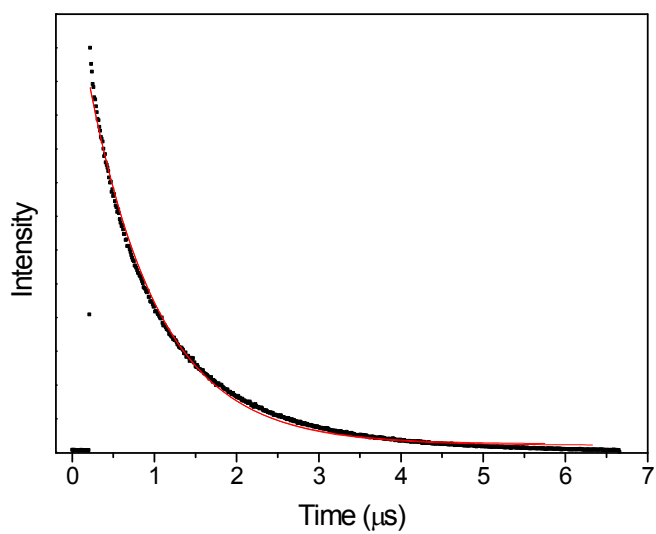


Figure 6S: Time-resolved decay curves of $fac-[Re(ampy)(CO)_3(bpy)]^+$ probed at maxima wavelength after 375 nm laser excitation in PMMA at 298 K.

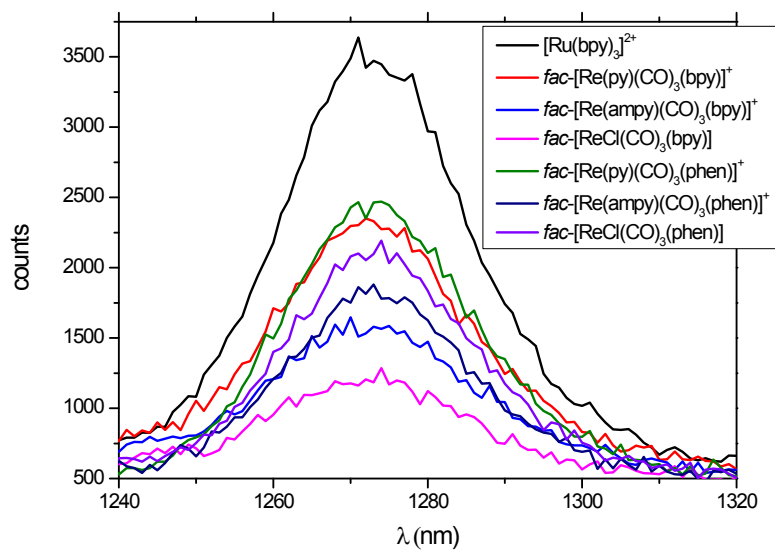


Figure 7S: Sensitized O_2 ($^1\Delta_g$) emission spectra generated by using rhenium(I) complexes after 375 nm laser excitation in CH_3CN at 298 K.

References

1. L. Agüero, L. G. Guerrero-Ramirez and I. Katime, *Mater. Sci. Appl.*, 2010, **1**, 103-108.
2. A. J. Dekoning, P. H. M. Budzelaar, J. Boersma and G. J. M. Vanderkerk, *Journal of Organometallic Chemistry*, 1980, **199**, 153-169.