

Luminescent Protein Staining with Re(I) Tetrazolato Complexes

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ESI – Electronic Supplementary Information

Table S1. Stretching frequencies (cm^{-1}) of the CO bands of all the Re(I) complexes reported in this work. Values are relative to solution state (dichloromethane as the solvent) IR spectra recorded at room temperature.

Complex	CO A'(1)	CO A'(2)/A''
<i>fac</i> -[Re(CO) ₃ (BCS)(Tph)] ²⁻	2029	1918
<i>fac</i> -[Re(CO) ₃ (BPS)(Tph)] ²⁻	2026	1914
<i>fac</i> -[Re(CO) ₃ (BC)(Tph)]	2022	1918
<i>fac</i> -[Re(CO) ₃ (BC)(Tph-Me)] ⁺	2037	1934

Figure S1: ESI-MS of *fac*-[Re(CO)₃(BCS)(Tph)]²⁻, negative region ions, CH₃OH.

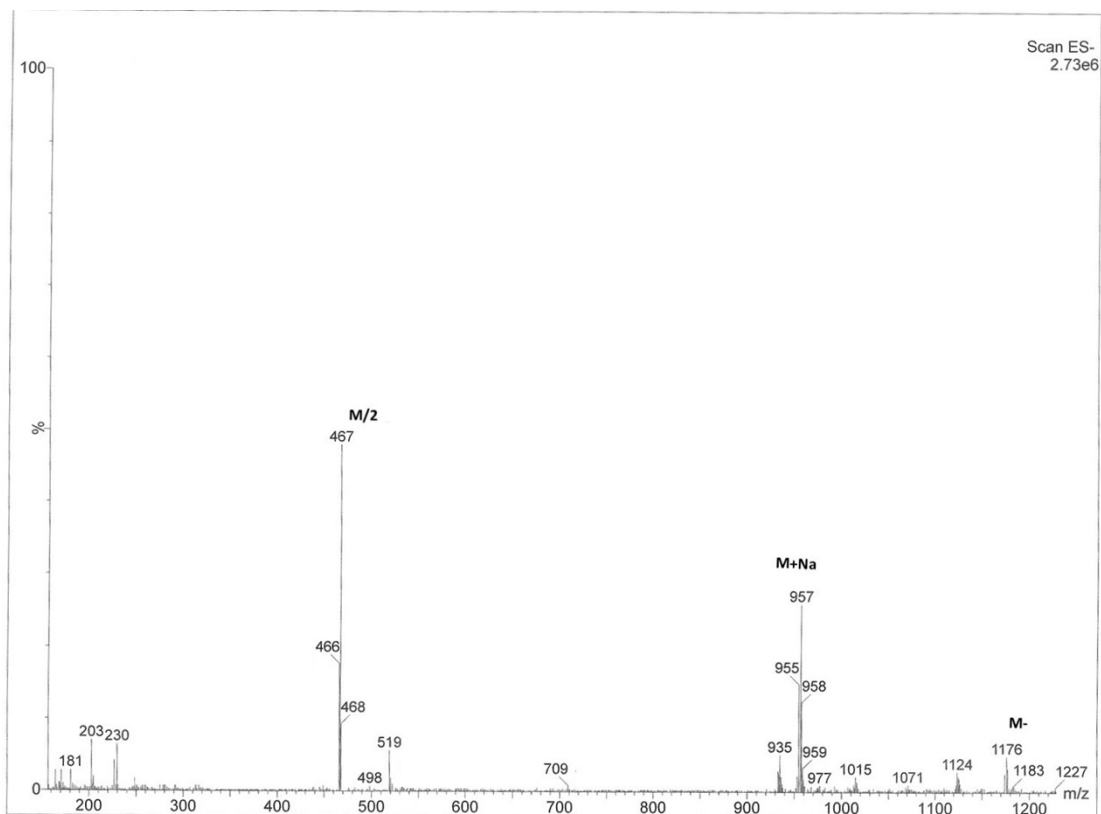


Figure S2: ESI-MS of *fac*-[Re(CO)₃(BPS)(Tph)]²⁻, negative region ions, CH₃OH.

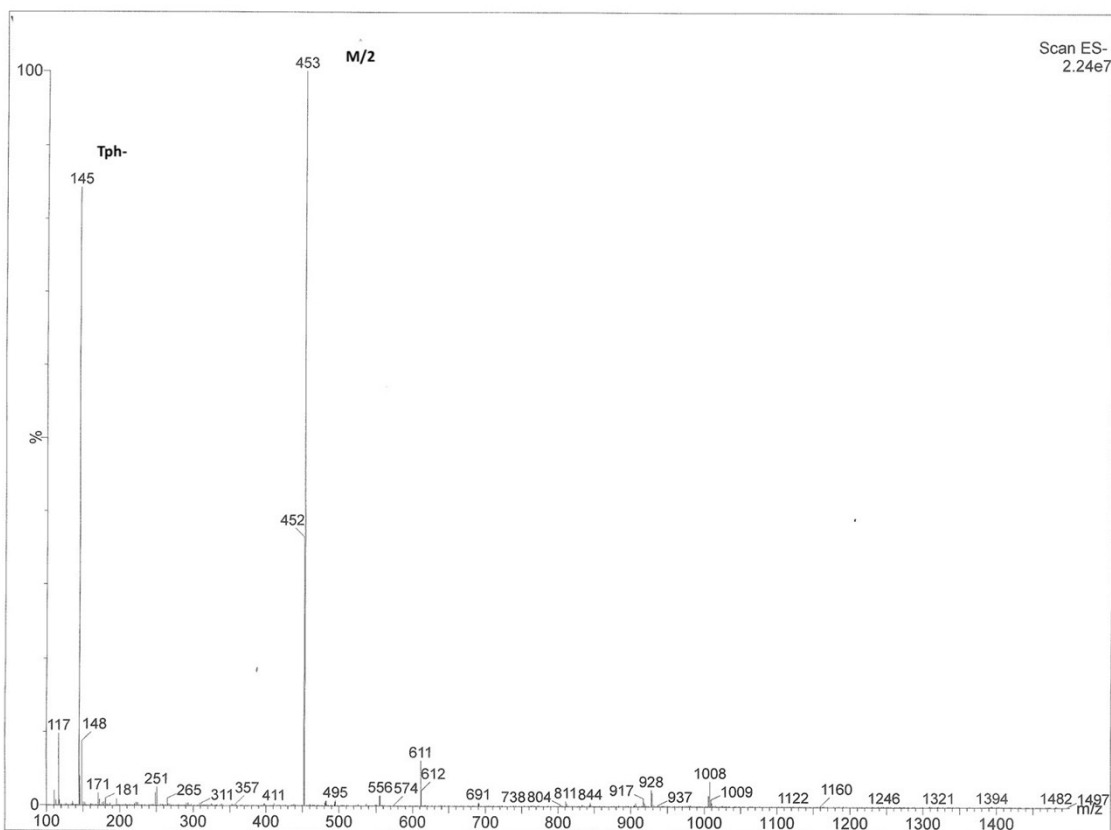


Figure S3: ESI-MS of *fac*-[Re(CO)₃(BC)(Tph)], positive region ions, CH₃CN.

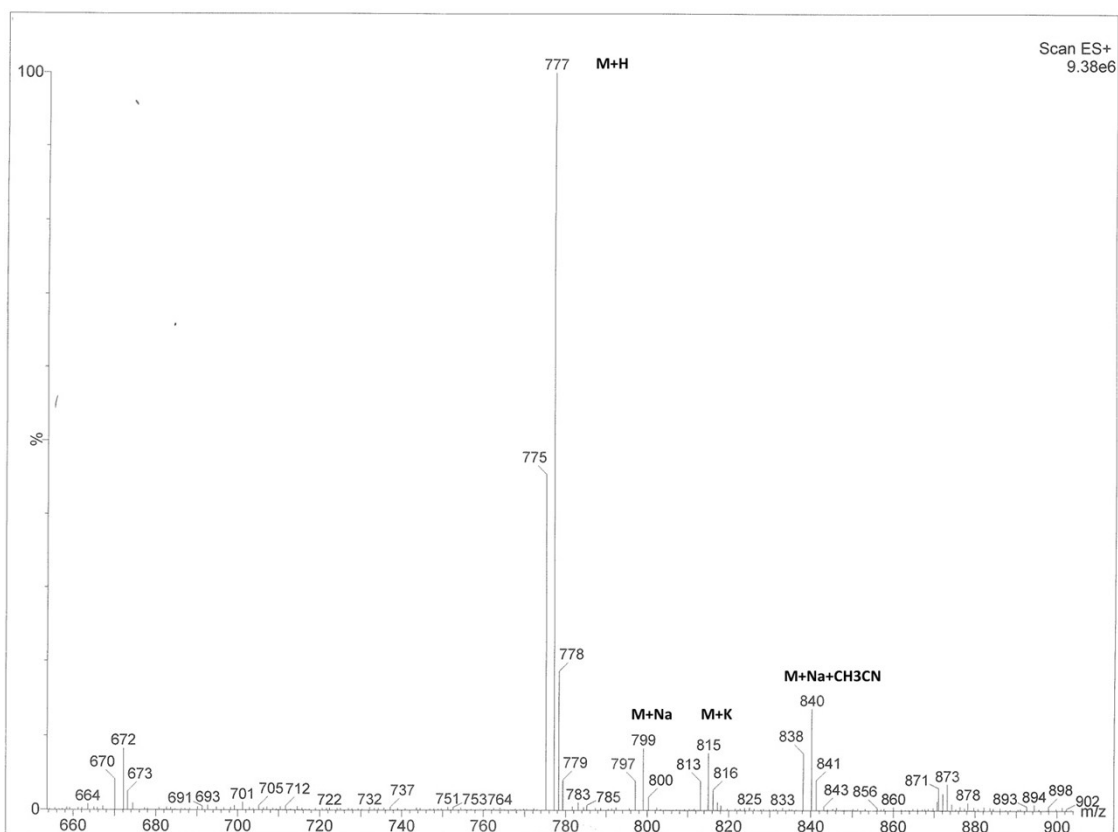


Figure S4: ESI-MS of *fac*-[Re(CO)₃(BC)(Tph-Me)]⁺, positive region ions, CH₃CN.

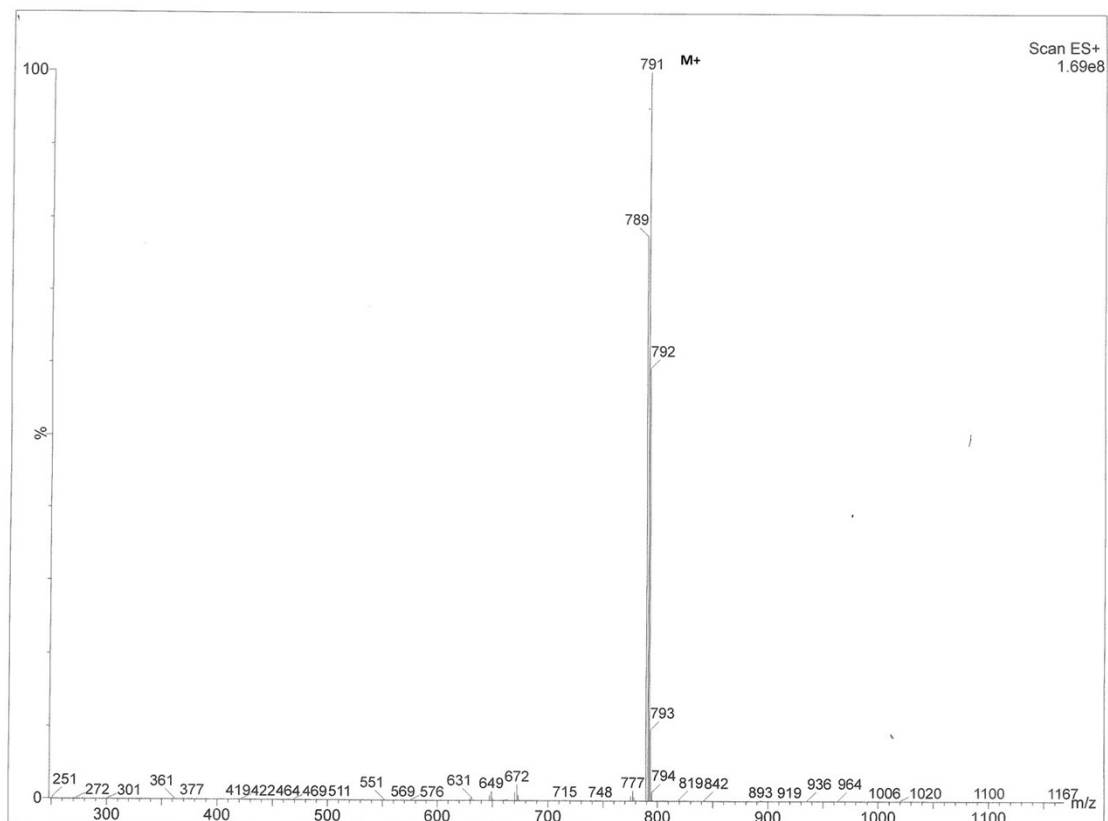


Figure S5: ^1H NMR of $\text{fac-}[\text{Re}(\text{CO})_3(\text{BCS})(\text{Tph})]^{2-}$, CD_3OD , 400 MHz, 298K.

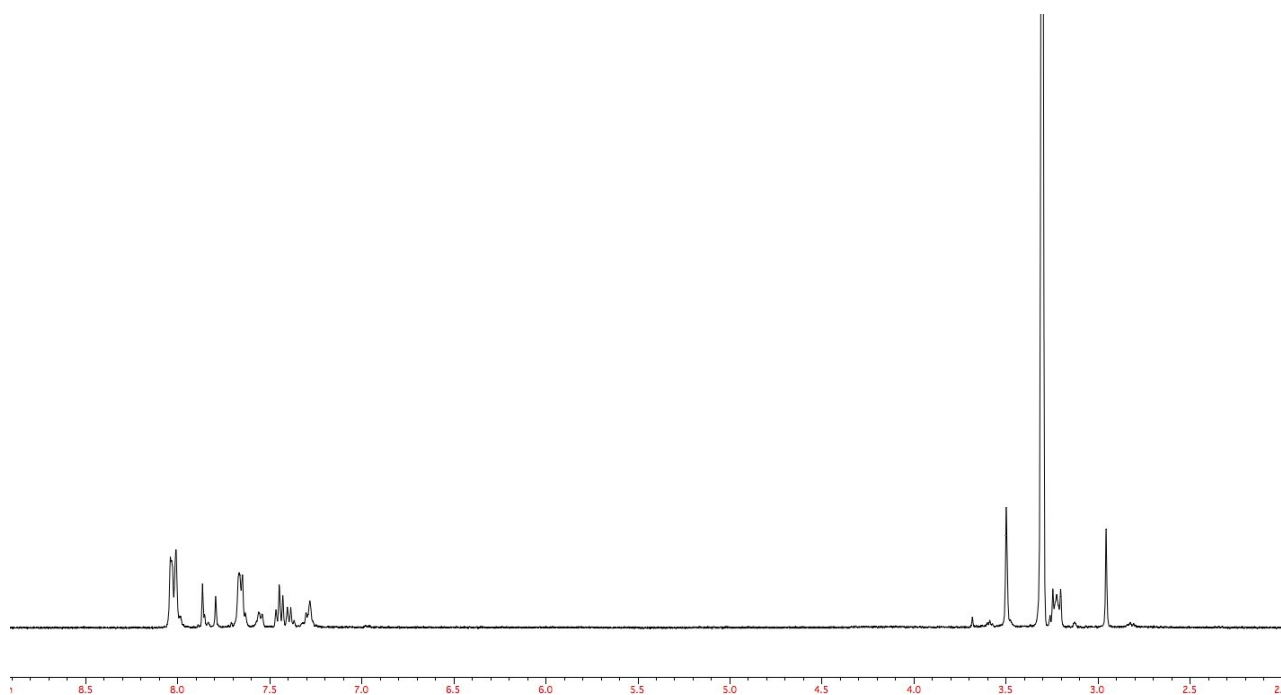


Figure S6: ^{13}C NMR of $\text{fac-}[\text{Re}(\text{CO})_3(\text{BCS})(\text{Tph})]^{2-}$, CD_3OD , 100 MHz, 298K.

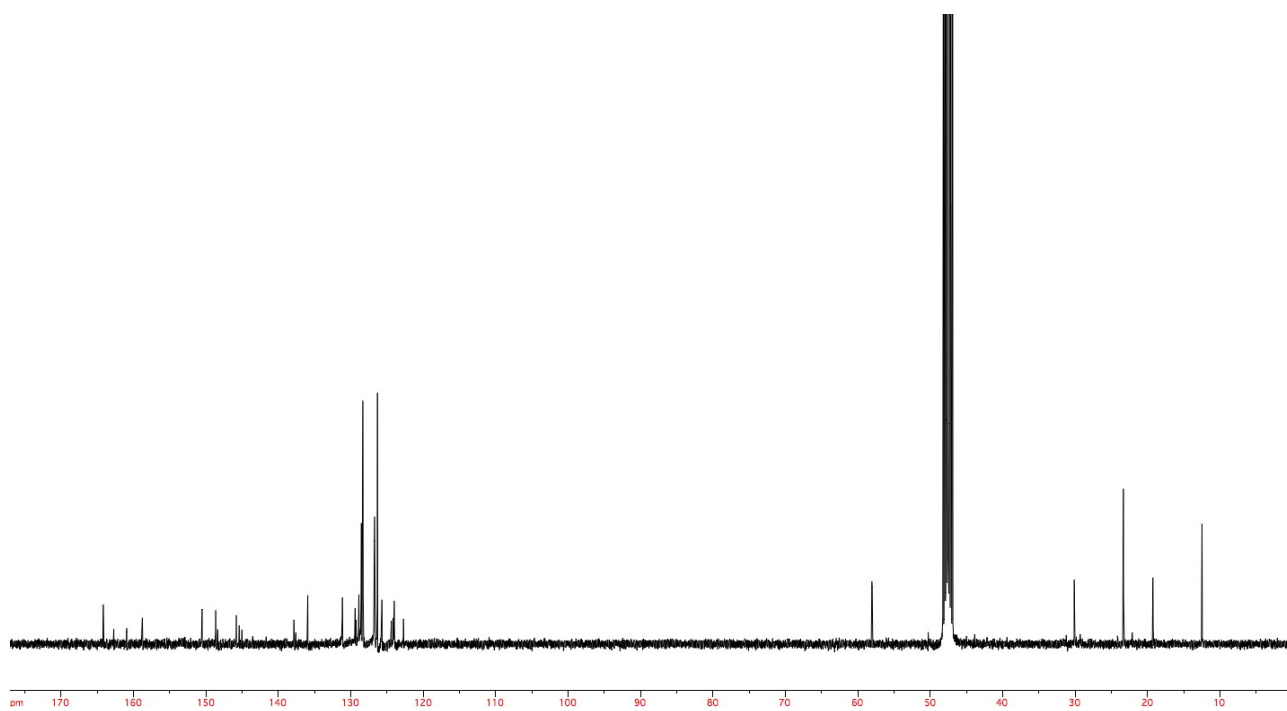


Figure S7: ^1H NMR of $\text{fac-}[\text{Re}(\text{CO})_3(\text{BPS})(\text{Tph})]^{2-}$, CD_3OD , 400 MHz, 298K.

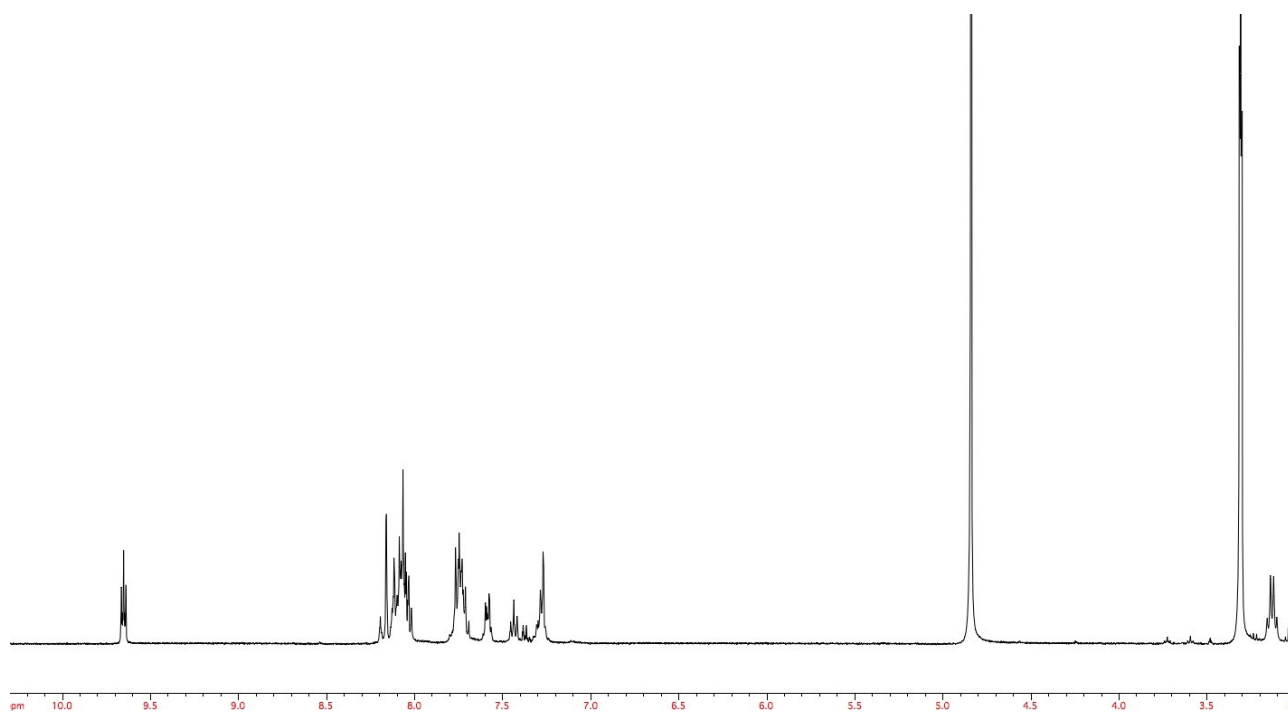


Figure S8: ^{13}C NMR of $\text{fac-}[\text{Re}(\text{CO})_3(\text{BPS})(\text{Tph})]^{2-}$, CD_3OD , 100 MHz, 298K.

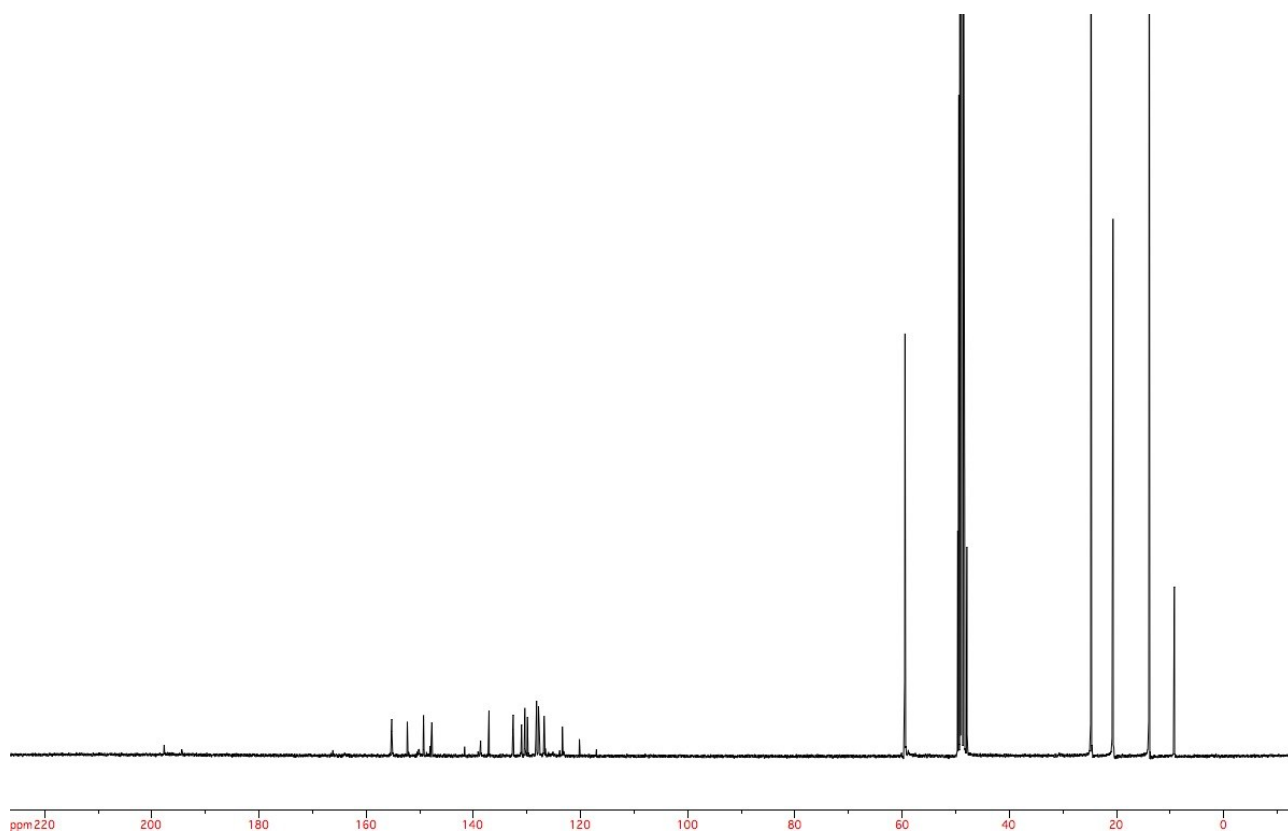


Figure S9: ^1H NMR of *fac*- $[\text{Re}(\text{CO})_3(\text{BC})(\text{Tph})]$, Acetone d^6 , 400 MHz, 298K.

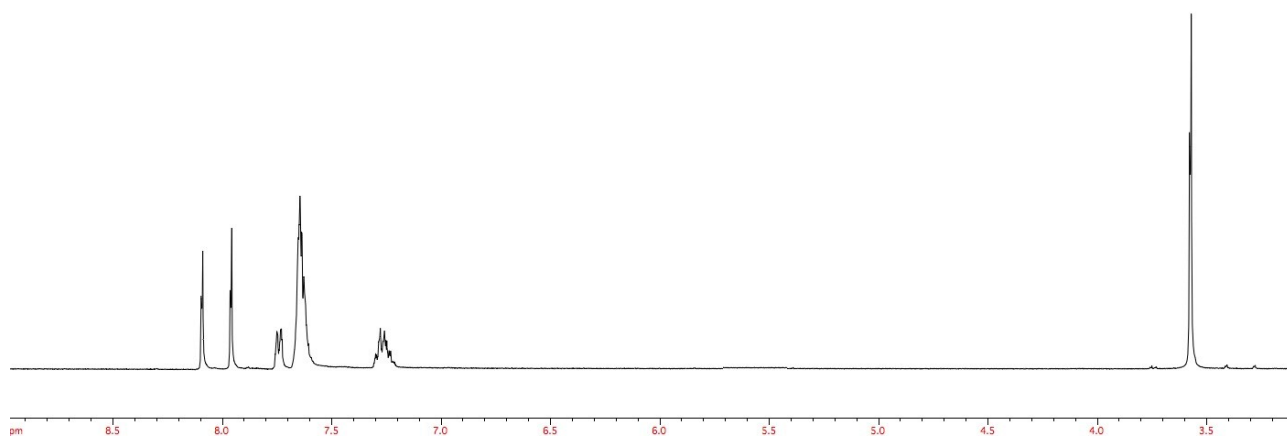


Figure S10: ^{13}C NMR of *fac*- $[\text{Re}(\text{CO})_3(\text{BC})(\text{Tph})]$, Acetone d^6 , 100 MHz, 298K.

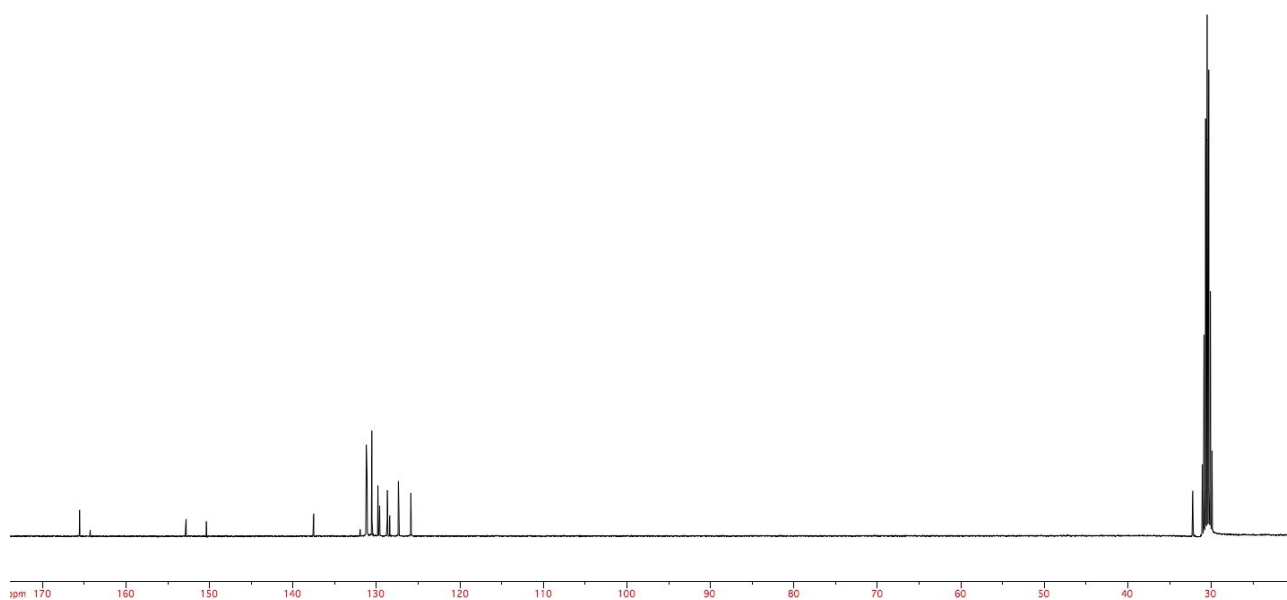


Figure S11: ^1H - ^1H COSY NMR of *fac*- $[\text{Re}(\text{CO})_3(\text{BC})(\text{Tph})]$, Acetone d_6 , 600 MHz, 298K.

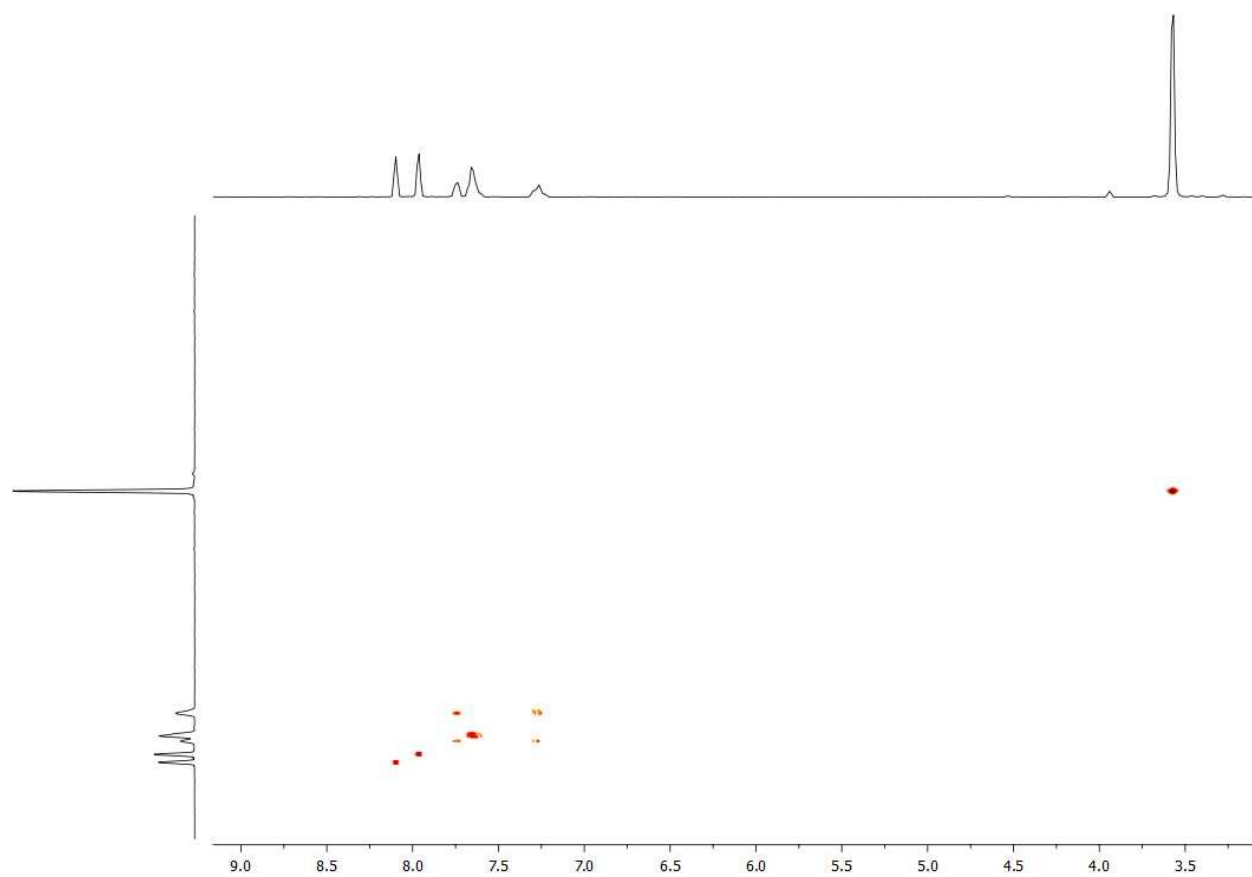


Figure S12: ^1H NMR of $\text{fac-}[\text{Re}(\text{CO})_3(\text{BC})(\text{Tph-Me})]^+$, Acetone d^6 , 400 MHz, 298K.

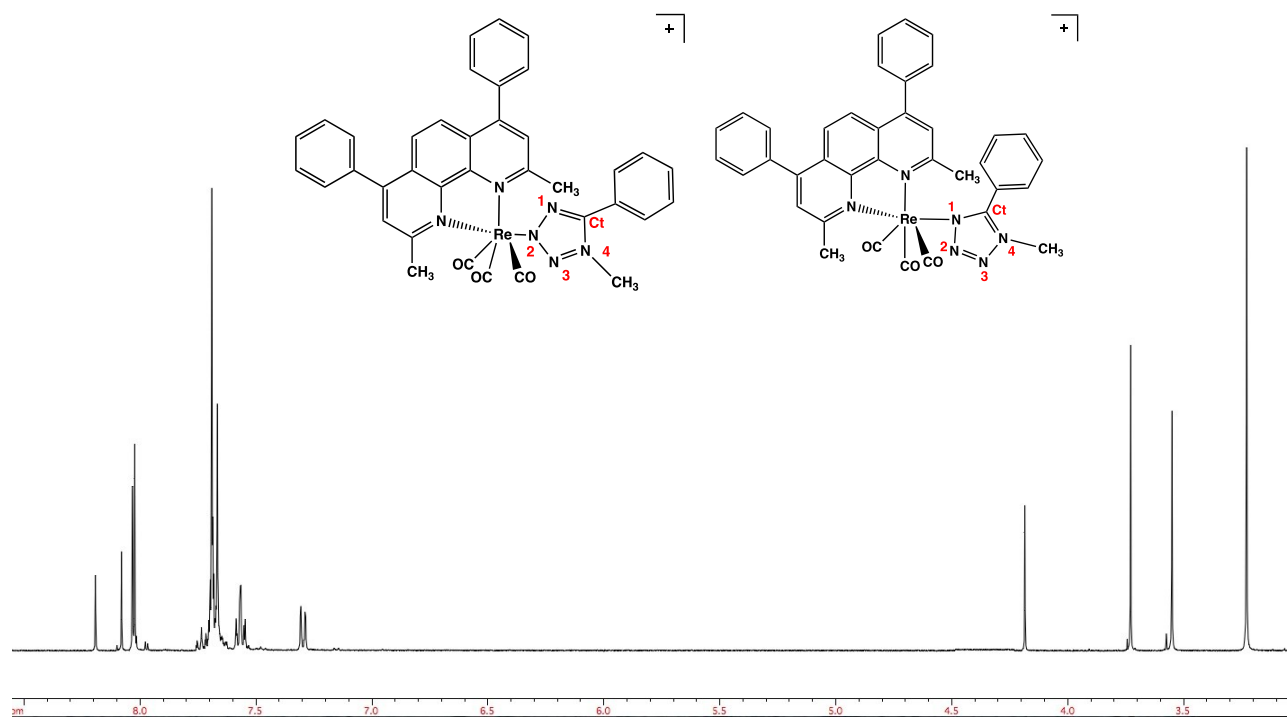


Figure S13: ^{13}C NMR of $\text{fac-}[\text{Re}(\text{CO})_3(\text{BC})(\text{Tph-Me})]^+$, Acetone d^6 , 100 MHz, 298K.

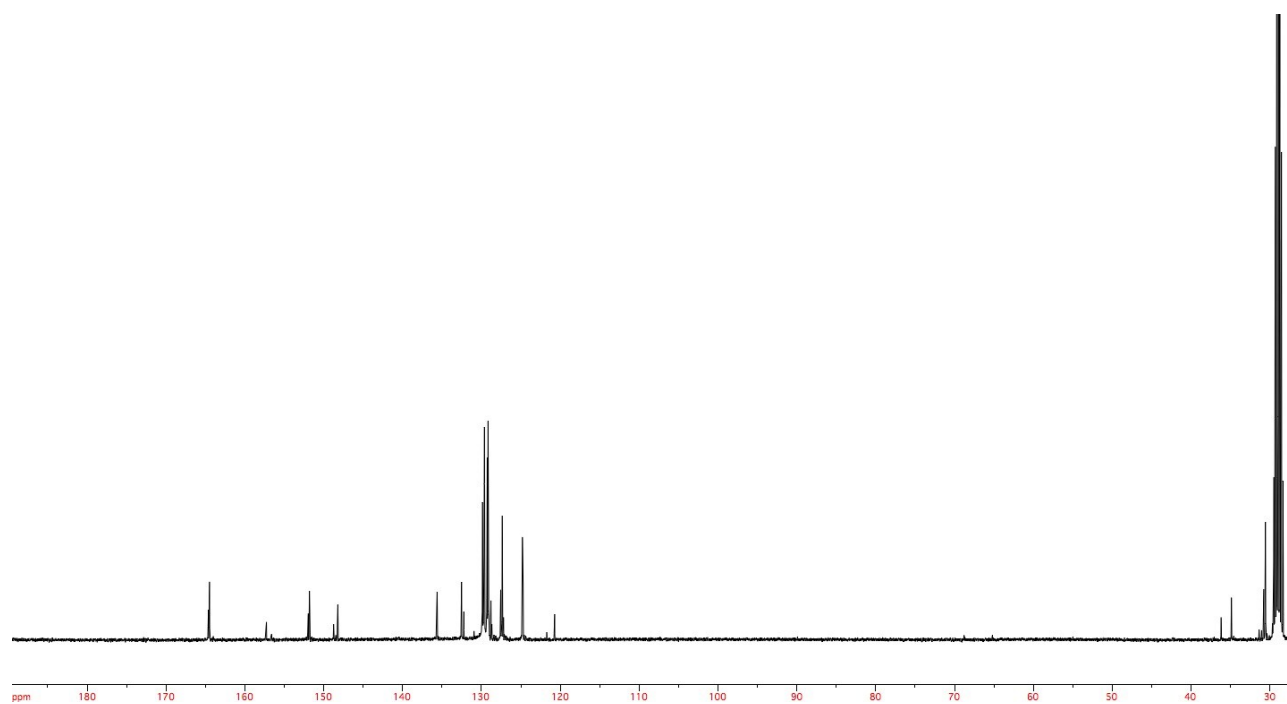


Figure S14: ^1H - ^1H COSY NMR of *fac*- $[\text{Re}(\text{CO})_3(\text{BC})(\text{Tph-Me})]^+$, Acetone d^6 , 600 MHz, 298K.

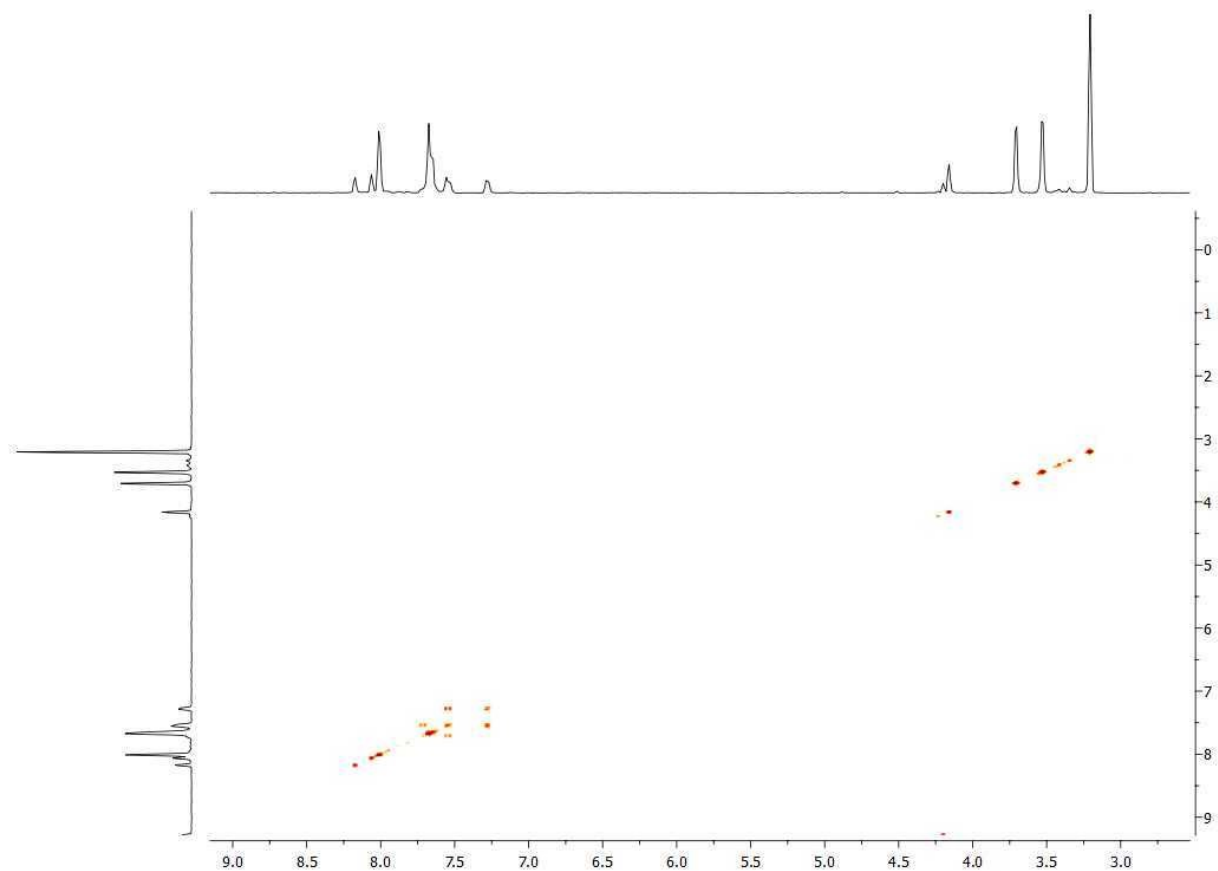


Figure S15: ^1H NMR and NOESY (overlay, 3.22 and 3.55 ppm) NMR of *fac*- $[\text{Re}(\text{CO})_3(\text{BC})(\text{Tph-Me})]^+$, Acetone d^6 , 400 MHz, 298K.

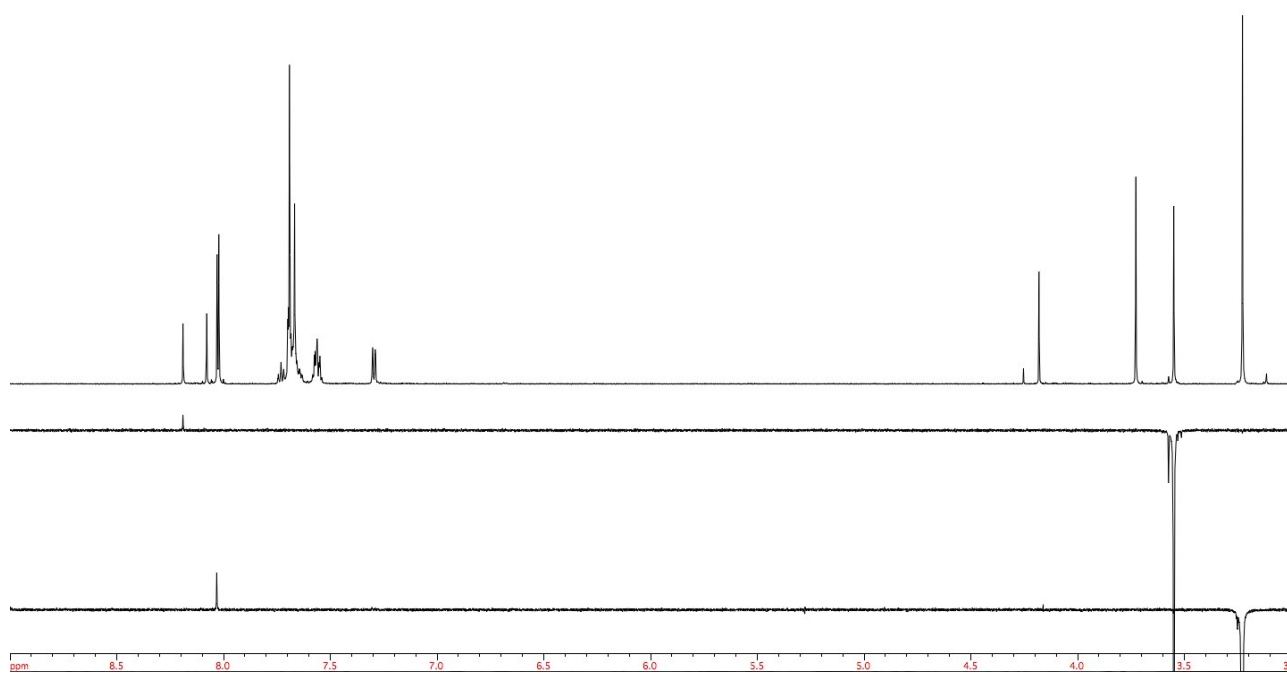


Figure S16: Absorption Profile of $fac-[Re(CO)_3(BCS)(Tph)]^{2-}$ in CH_3OH (red line) and H_2O (blue line), $10^{-5}M$, 298K.

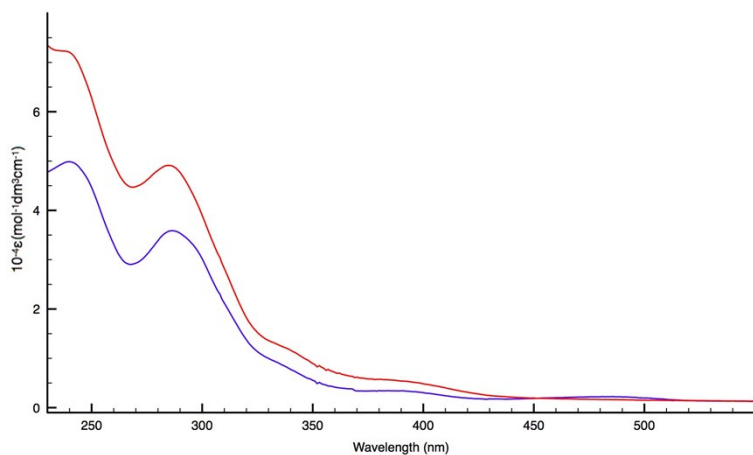


Figure S17: Emission Profile of $fac-[Re(CO)_3(BCS)(Tph)]^{2-}$ air-equilibrated (black line) and deoxygenated solution (blue line), $10^{-5}M$, CH_3OH , 298K.

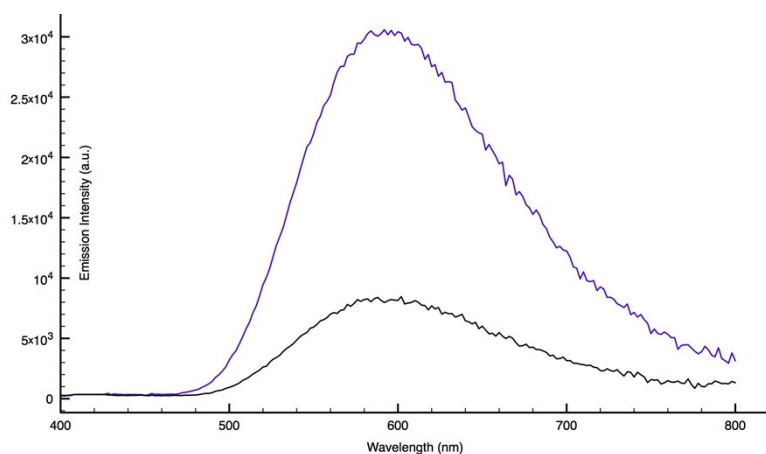


Figure S18: Emission Profile of $fac-[Re(CO)_3(BCS)(Tph)]^{2-}$ air-equilibrated (black line) and deoxygenated solution (blue line), $10^{-5}M$, H_2O , 298K.

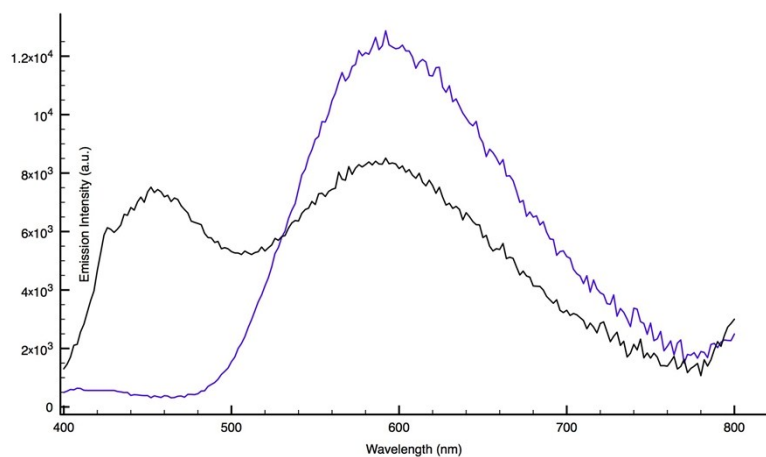


Figure S19: Emission Map of $fac-[Re(CO)_3(BCS)(Tph)]^{2-}$, $10^{-5}M$, H₂O, 298K.

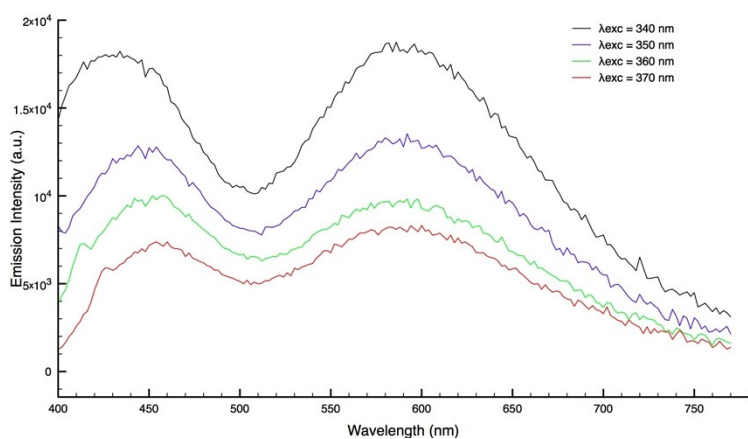


Figure S20: Excitation Profile of $fac-[Re(CO)_3(BCS)(Tph)]^{2-}$ CH₃OH (black line) H₂O (blue line), $10^{-5}M$, CH₃OH, 298K.

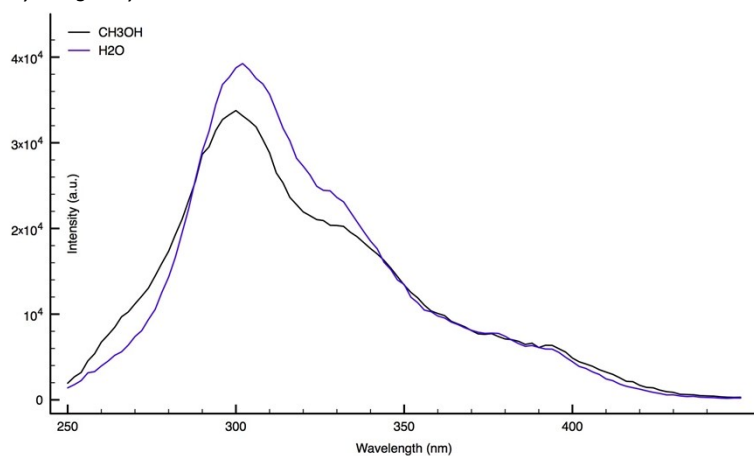


Figure S21: Emission Profile of $fac-[Re(CO)_3(BCS)(Tph)]^{2-}$, $10^{-5}M$, CH₃OH, 77K.

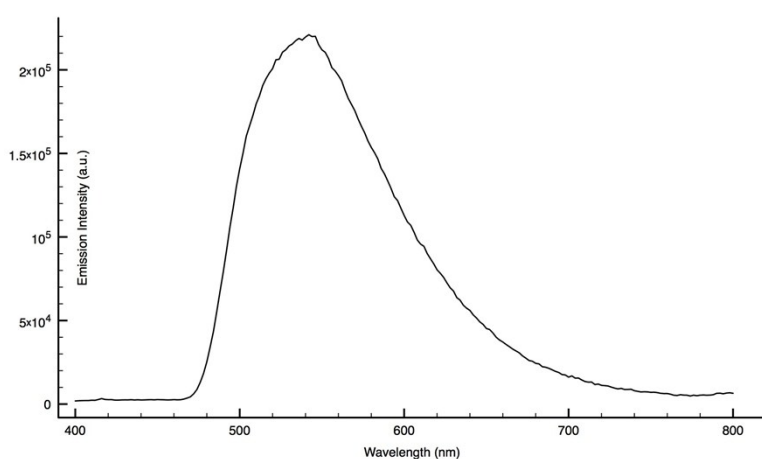


Figure S22: Absorption Profile of $fac-[Re(CO)_3(BPS)(Tph)]^{2-}$ in CH_2Cl_2 (red line) and H_2O (blue line), $10^{-5}M$, 298K.

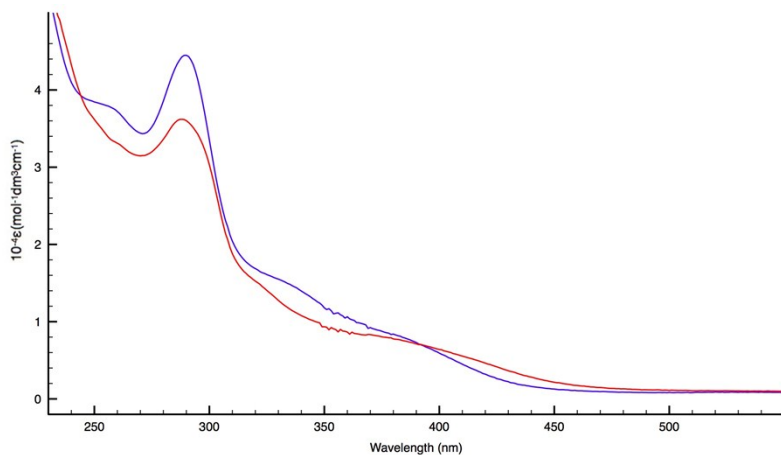


Figure S23: Emission Profile of $fac-[Re(CO)_3(BPS)(Tph)]^{2-}$ air-equilibrated (black line) and deoxygenated solution (blue line), $10^{-5}M$, CH_2Cl_2 , 298K.

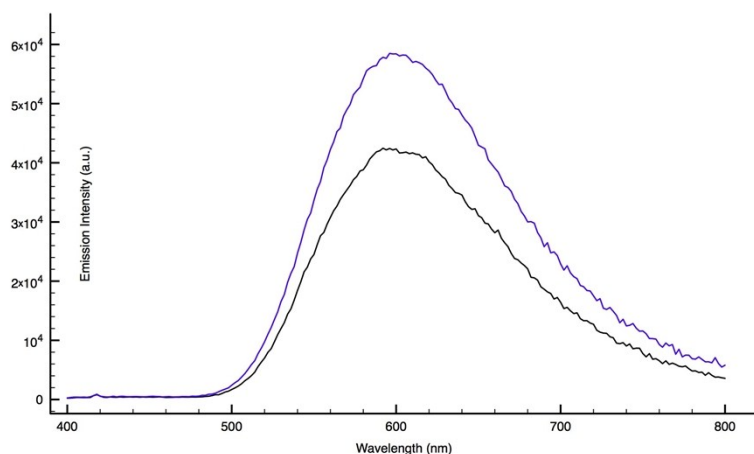


Figure S24: Emission Profile of $fac-[Re(CO)_3(BPS)(Tph)]^{2-}$, $10^{-5}M$, H_2O , 298K.

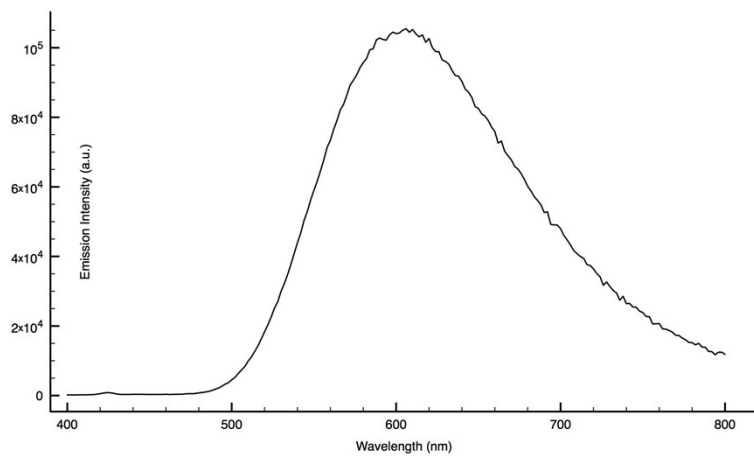


Figure S25: Excitation Profile of *fac*-[Re(CO)₃(BPS)(Tph)]²⁻ CH₂Cl₂ (black line) H₂O (blue line), 10⁻⁵M, CH₃OH, 298K.

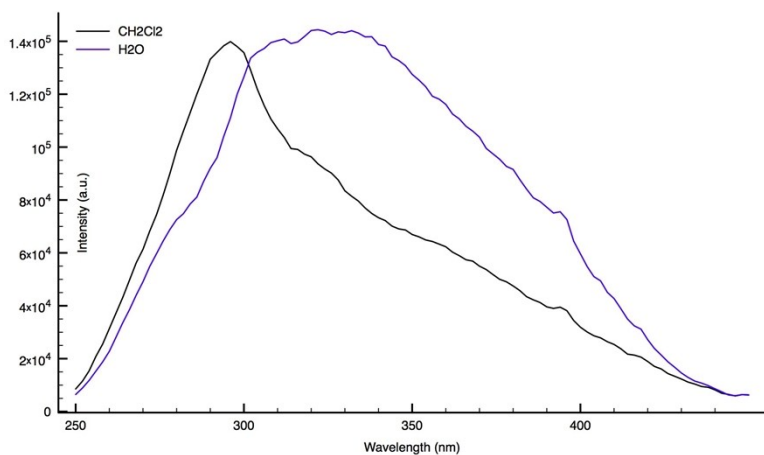


Figure S26: Emission Profile of *fac*-[Re(CO)₃(BPS)(Tph)]²⁻, 10⁻⁵M, CH₂Cl₂, 77K.

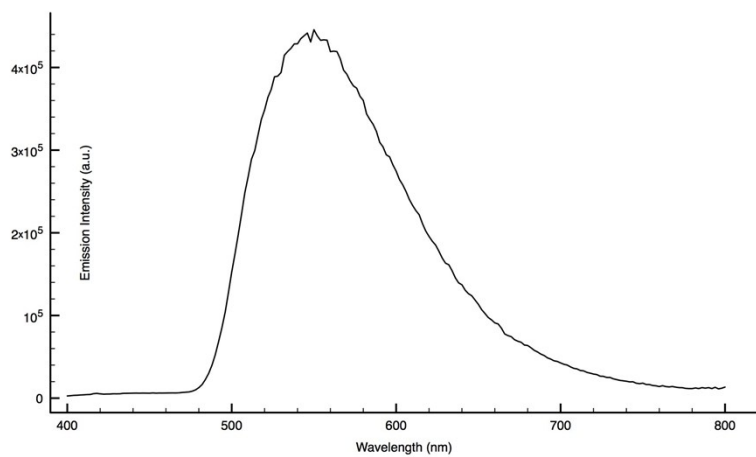


Figure S27: Absorption Profile of *fac*-[Re(CO)₃(BC)(Tph)] 10⁻⁵M, CH₂Cl₂, 298K.

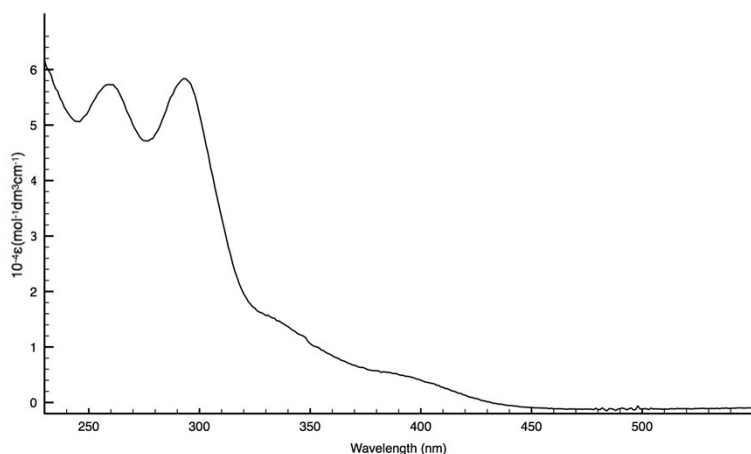


Figure S28: Emission Profile of *fac*-[Re(CO)₃(BC)(Tph)] air-equilibrated (black line) and deoxygenated solution (blue line), 10⁻⁵M, CH₂Cl₂, 298K.

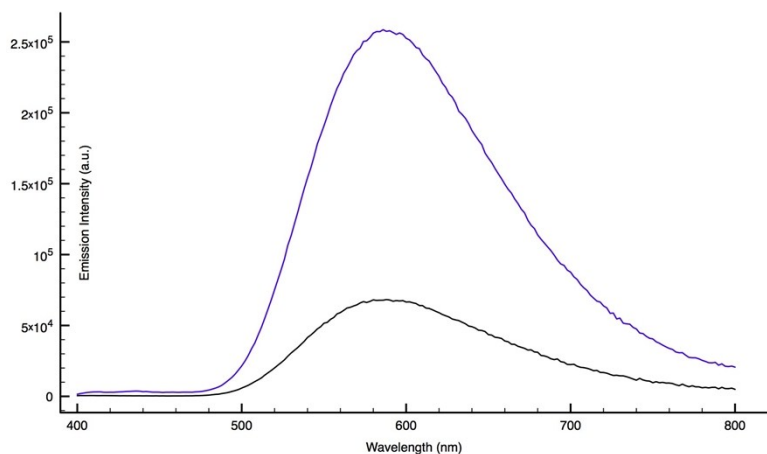


Figure S29: Excitation Profile of *fac*-[Re(CO)₃(BC)(Tph)] 10⁻⁵M, CH₂Cl₂, 298K.

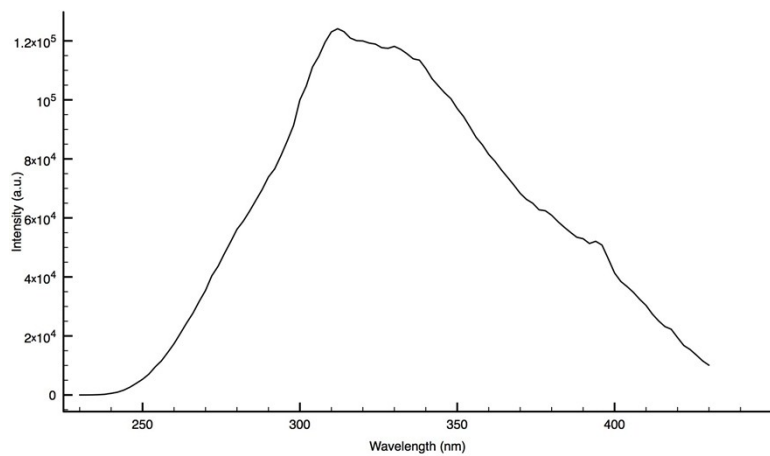


Figure S30: Emission Profile of *fac*-[Re(CO)₃(BC)(Tph)], $\lambda_{\text{exc}} = 370 \text{ nm}$, 10^{-5}M , CH₂Cl₂, 298K.

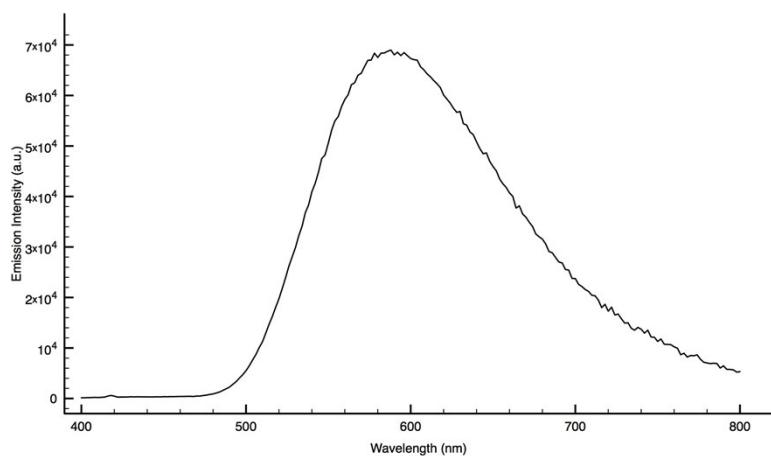


Figure S31: Emission Profile of *fac*-[Re(CO)₃(BC)(Tph)], $\lambda_{\text{exc}} = 302 \text{ nm}$, 10^{-5}M , CH₂Cl₂, 298K.

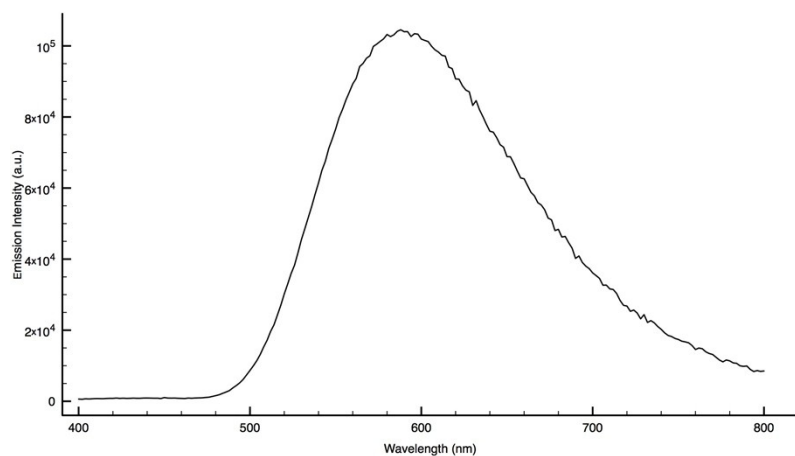


Figure S32: Emission Profile of *fac*-[Re(CO)₃(BC)(Tph)], 10^{-5}M , CH₂Cl₂, 77K.

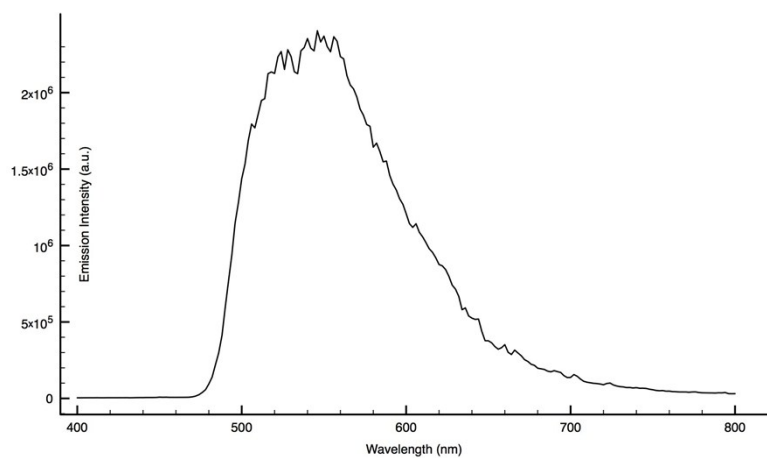


Figure S33: Absorption Profile of *fac*-[Re(CO)₃(BC)(Tph-Me)]⁺ 10⁻⁵M, CH₂Cl₂, 298K.

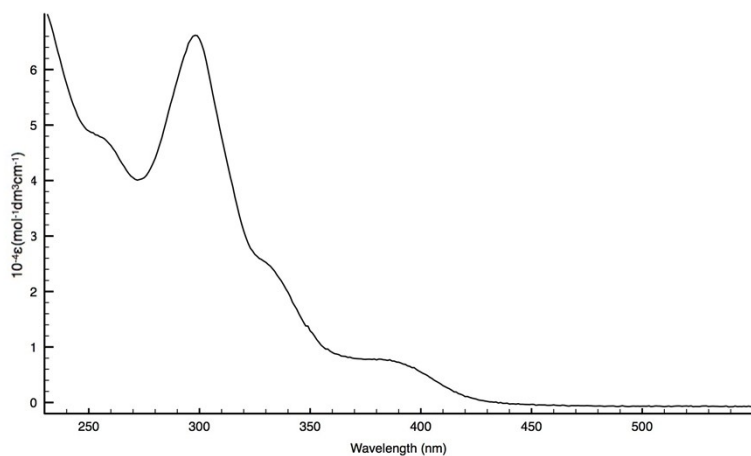


Figure S34: Emission Profile of *fac*-[Re(CO)₃(BC)(Tph-Me)]⁺ air-equilibrated (black line) and deoxygenated solution (blue line), 10⁻⁵M, CH₂Cl₂, 298K.

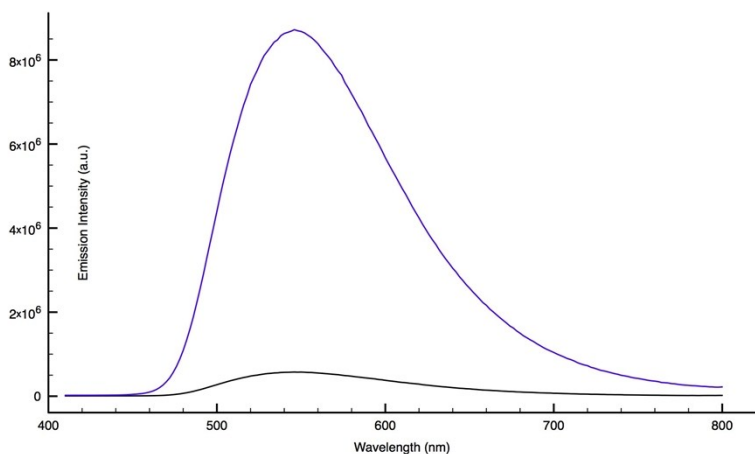


Figure S35: Excitation Profile of *fac*-[Re(CO)₃(BC)(Tph-Me)]⁺ 10⁻⁵M, CH₂Cl₂, 298K.

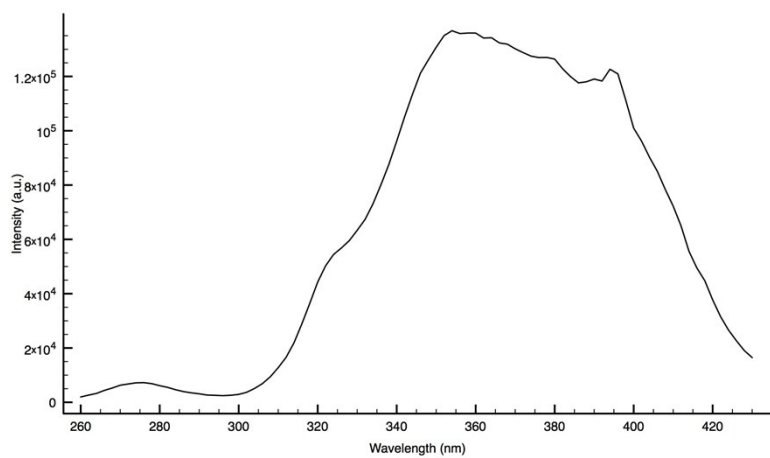


Figure S36: Emission Profile of $fac\text{-[Re(CO)}_3\text{(BC)(Tph-Me)]}^+$, $\lambda_{\text{exc}} = 370 \text{ nm}$, 10^{-5}M , CH_2Cl_2 , 298K.

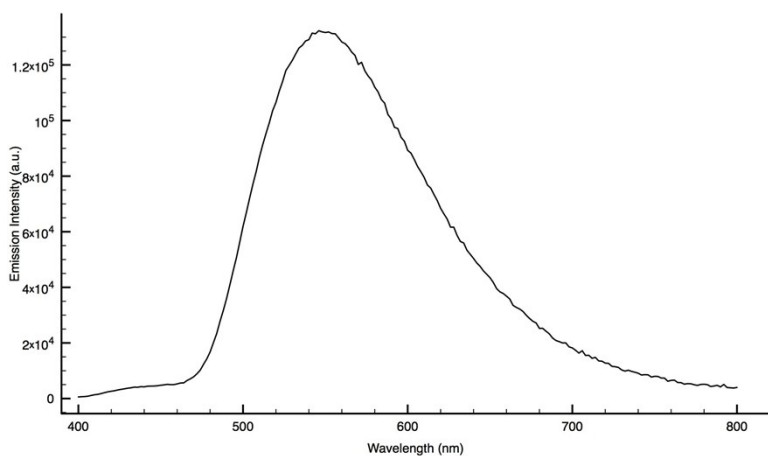


Figure S37: Emission Profile of $fac\text{-[Re(CO)}_3\text{(BC)(Tph-Me)]}^+$, $\lambda_{\text{exc}} = 302 \text{ nm}$, 10^{-5}M , CH_2Cl_2 , 298K.

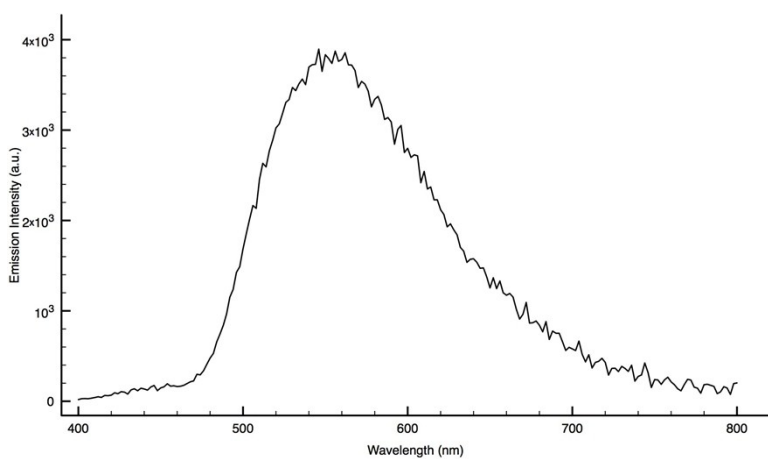


Figure S38: Emission Profile of $fac\text{-[Re(CO)}_3\text{(BC)(Tph-Me)]}^+$ ($\lambda_{\text{exc}} = 370 \text{ nm}$ blue line) and $fac\text{-[Re(CO)}_3\text{(BC)(Tph-Me)]}^+$ ($\lambda_{\text{exc}} = 302 \text{ nm}$ black line), 10^{-5}M , CH_2Cl_2 , 298K.

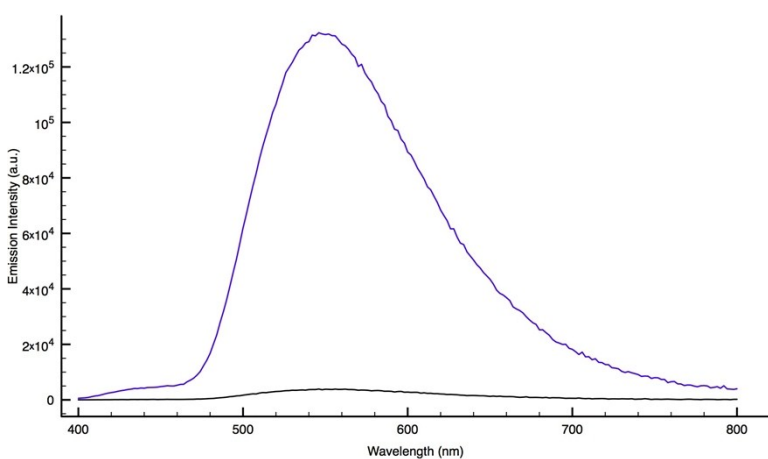


Figure S39: Emission Profile of $fac-[Re(CO)_3(BC)(Tph-Me)]^+$, $10^{-5}M$, CH_2Cl_2 , 77K.

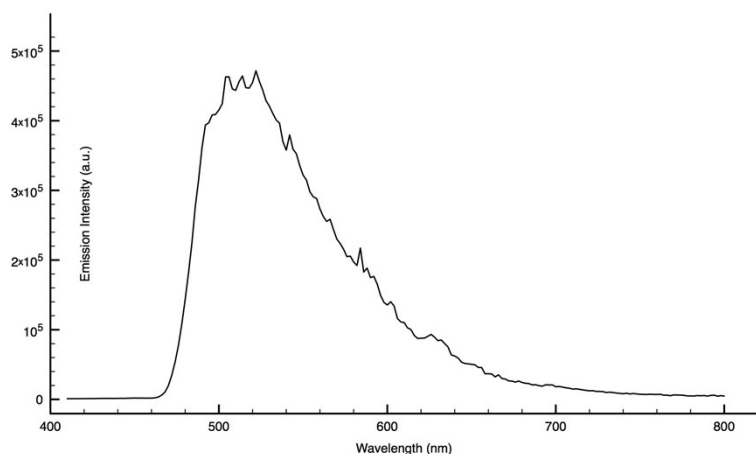


Figure S40: Excitation Profile of $fac-[Re(CO)_3(BC)(Tph)]$ (black line) and $fac-[Re(CO)_3(BC)(Tph-Me)]^+$ (blue line), $10^{-5}M$, CH_2Cl_2 , 298K.

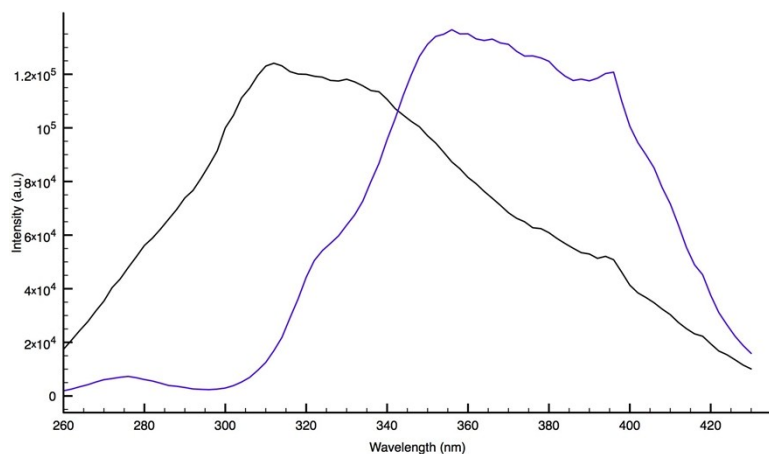


Figure S41: Normalized Emission Profile of $fac-[Re(CO)_3(BC)(Tph)]$ (black line) and $fac-[Re(CO)_3(BC)(Tph-Me)]^+$ (blue line), $10^{-5}M$, CH_2Cl_2 , 298K.

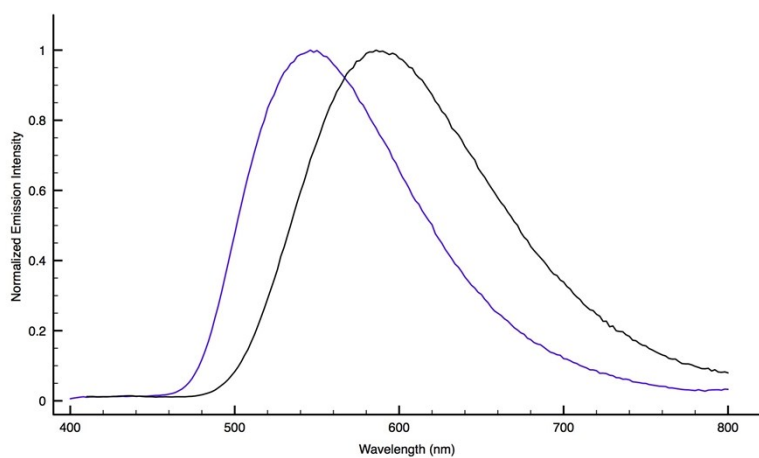


Table S2 - Crystal data and collection details for *fac*-[Re(CO)₃(BC)(Tph)].

Formula	C ₃₆ H ₂₅ N ₆ O ₃ Re
Fw	775.82
T, K	100(2)
λ , Å	0.71073
Crystal system	Orthorhombic
Space Group	<i>Pbca</i>
a, Å	10.9090(8)
b, Å	22.6914(18)
c, Å	24.2243(19)
Cell Volume, Å ³	5996.5(8)
Z	8
D _c , g cm ⁻³	1.719
μ , mm ⁻¹	4.102
F(000)	3056
Crystal size, mm	0.16×0.13×0.12
θ limits, °	1.681–26.999
Index ranges	-13 ≤ h ≤ 13 -28 ≤ k ≤ 28 -30 ≤ l ≤ 30
Reflections collected	81467
Independent reflections	6538 [<i>R</i> _{int} = 0.0493]
Completeness to θ max	100.0%
Data / restraints / parameters	6538 / 0 / 417
Goodness on fit on F ²	1.189
R ₁ (<i>I</i> > 2 σ (<i>I</i>))	0.0333
wR ₂ (all data)	0.0548
Largest diff. peak and hole, e Å ⁻³	1.069 / -2.060