

SUPPORT INFORMATION

Spectroscopic characterization of a new Re(I) tricarbonyl complex with a thiosemicarbazone derivative: towards sensing and electrocatalytic applications

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Figure S1. Photo of the homemade H-cell employed in the CPE experiments for CO₂ reduction

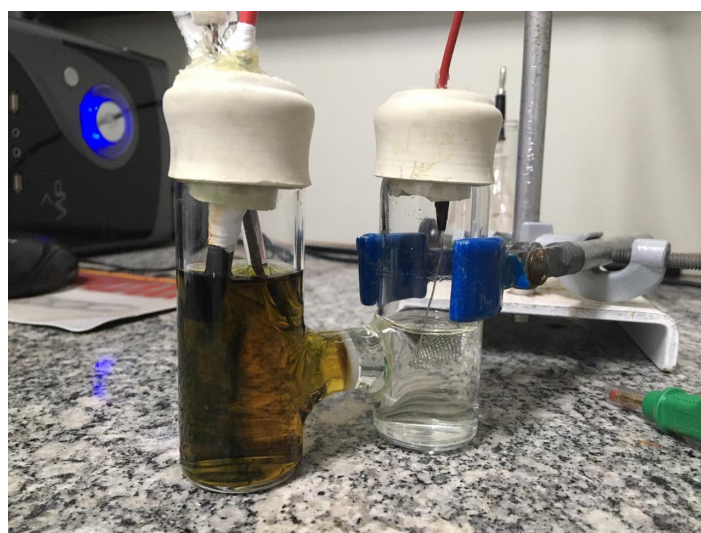


Figure S2. ATR FTIR of (A) phet e (B) *fac*-[ReCl(CO)₃(phet)].

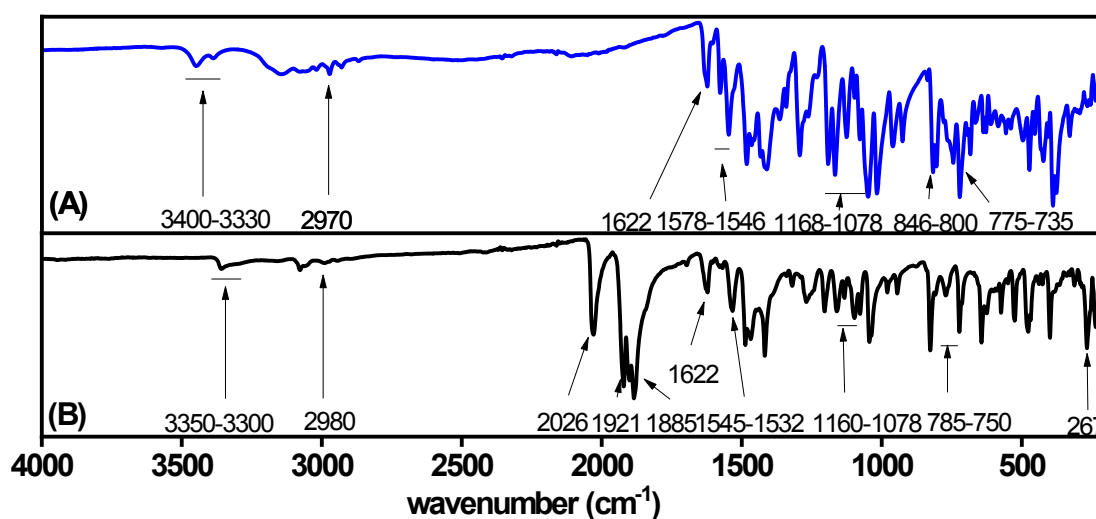


Figure S3 ^1H -RMN of free phet and *fac*-[ReCl(CO)₃(phet)] in DMSO d₆; 400 MHz.

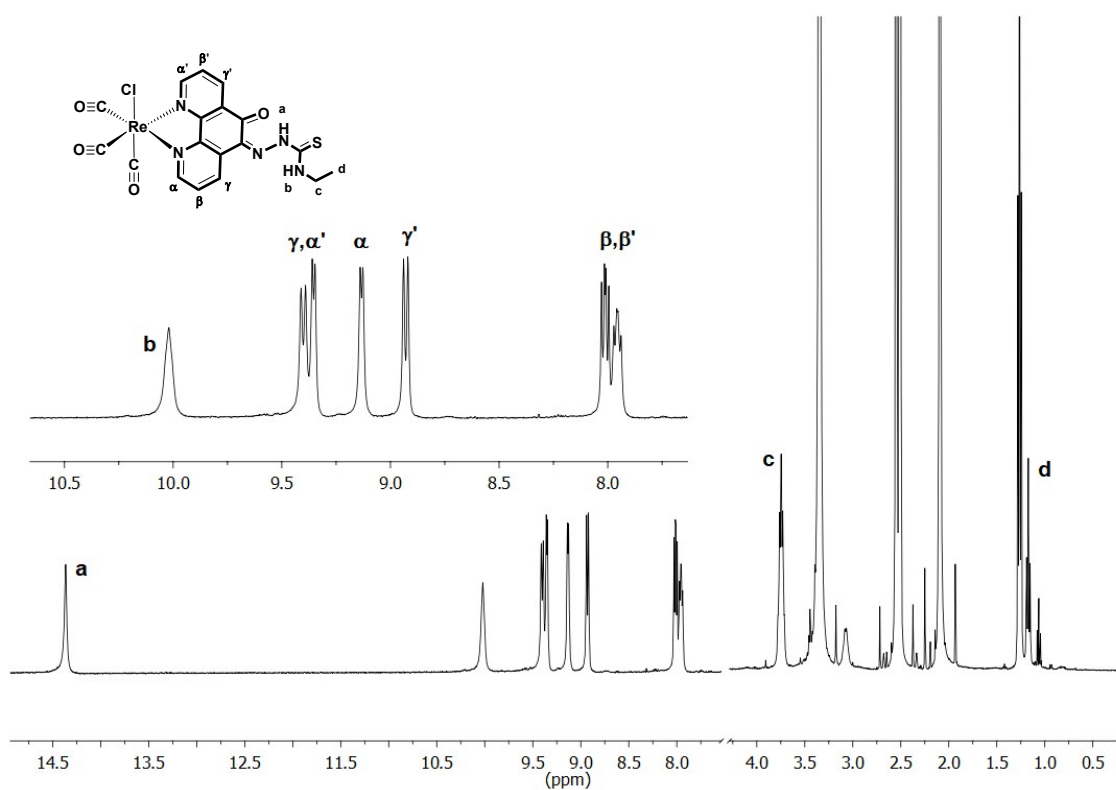
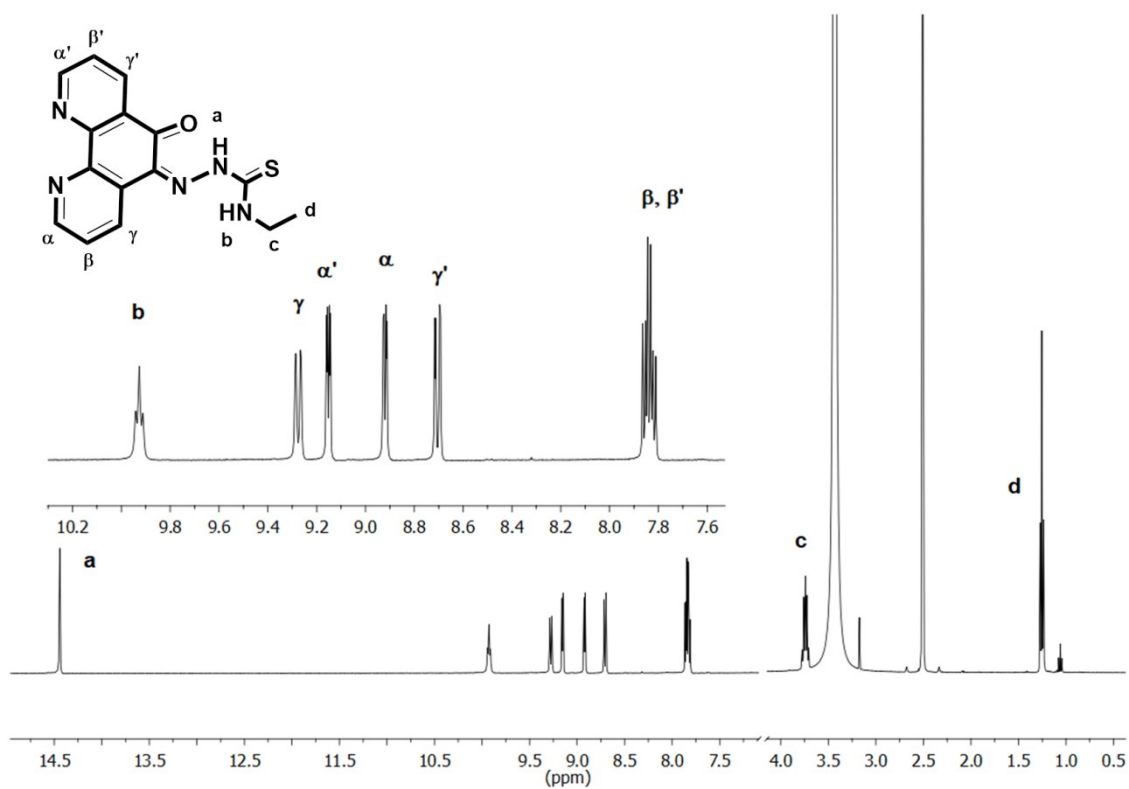


Figure S4. H-H COSY spectrum of phet and *fac*-[ReCl(CO)₃(phet)] in , DMSO d₆, 400 MHz.

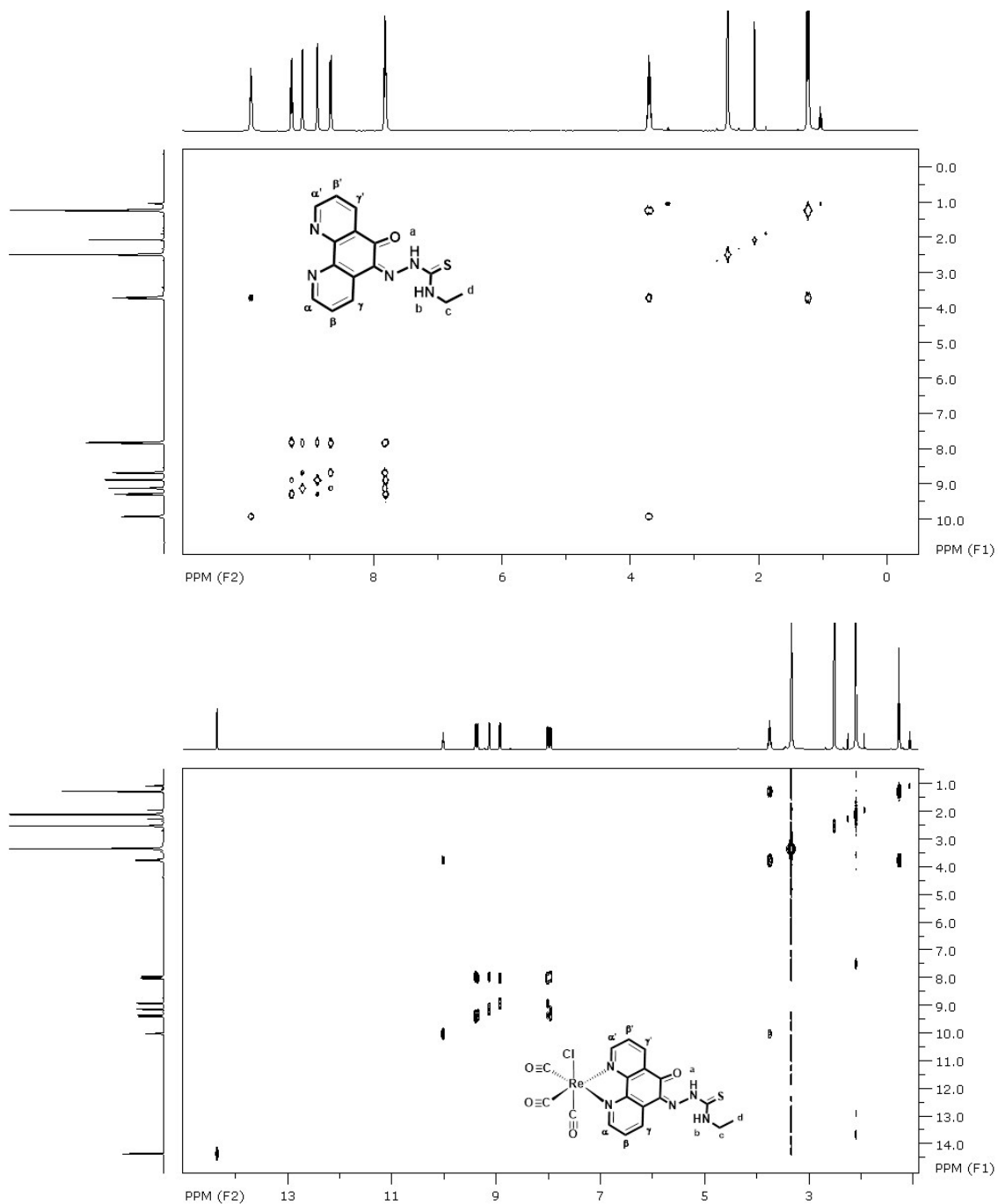


Figure S5. HMBC spectrum of phet in DMSO d₆, 400 MHz.

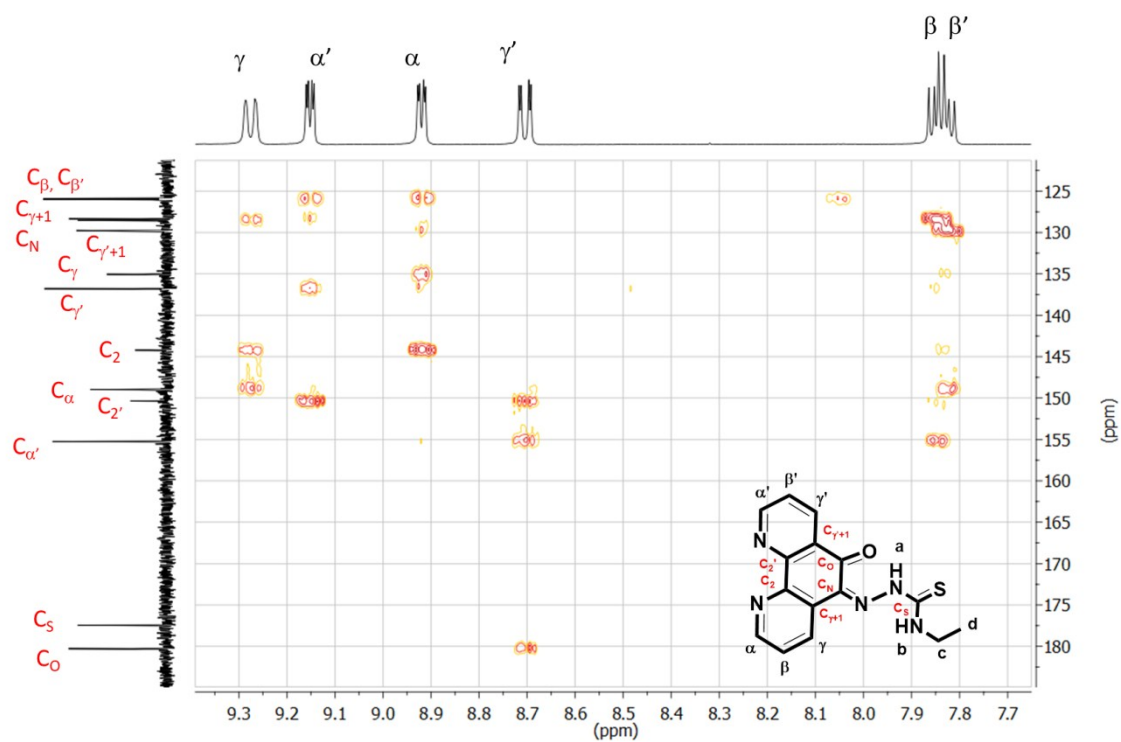


Figure S6. HSQC spectrum of phet in DMSO d₆, 400 MHz.

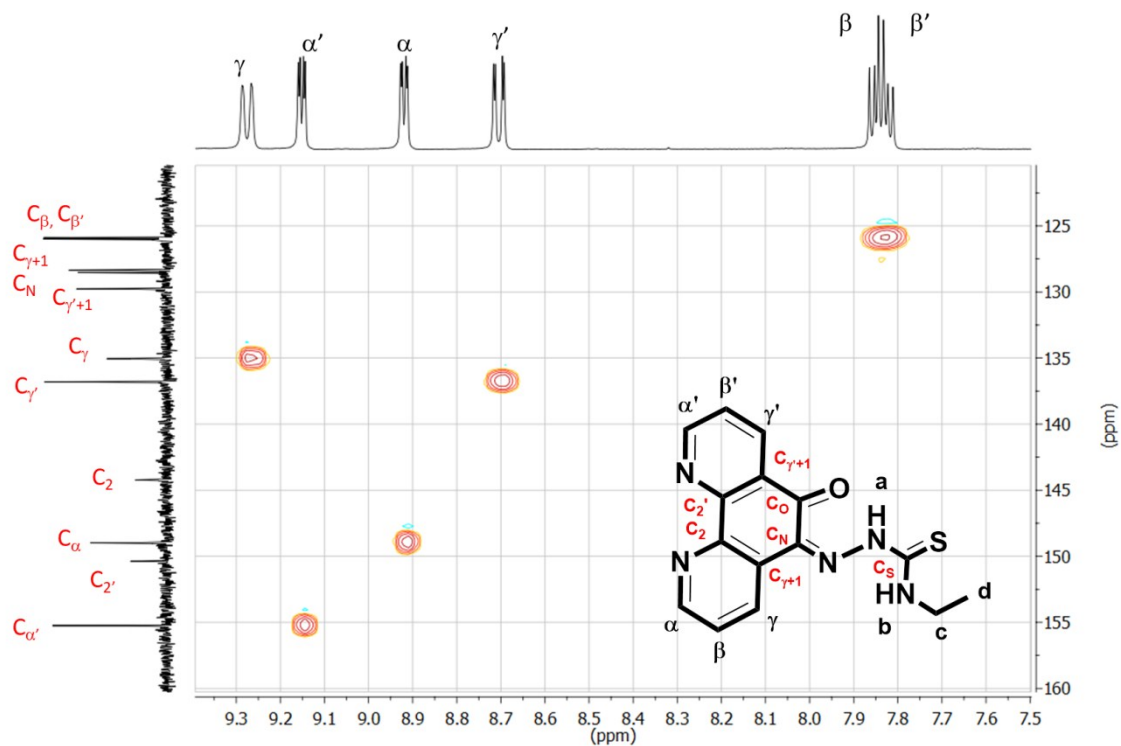


Figure S7. Isosurface plots of molecular orbitals of phet and *fac*-[ReCl(CO)₃(phet)].

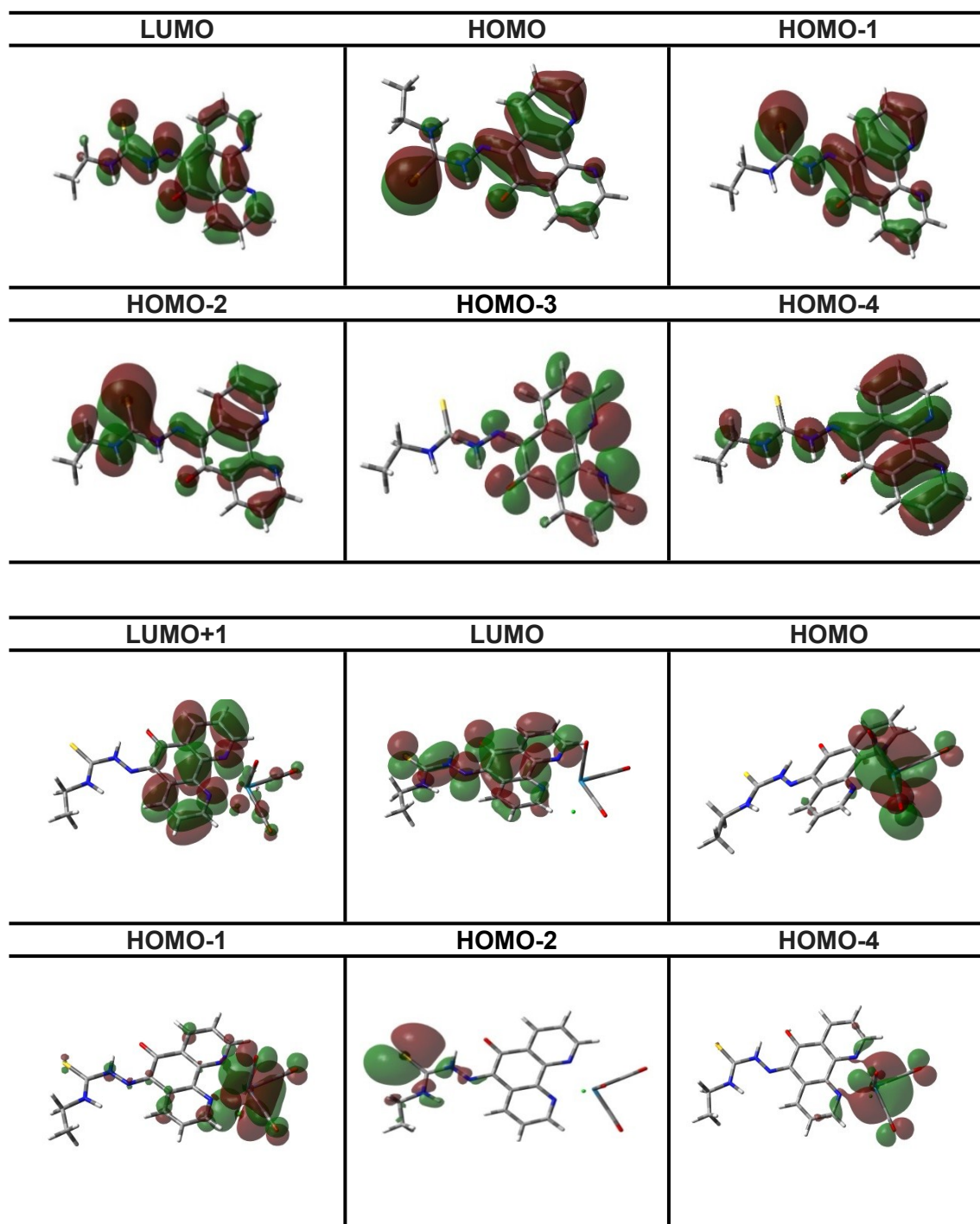


Figure S8. Theoretical (---) and experimental (—) in Acetonitrile electronic spectra of *fac*-[ReCl(CO)₃(phet)]. The bars correspond to the calculated oscillator strength.

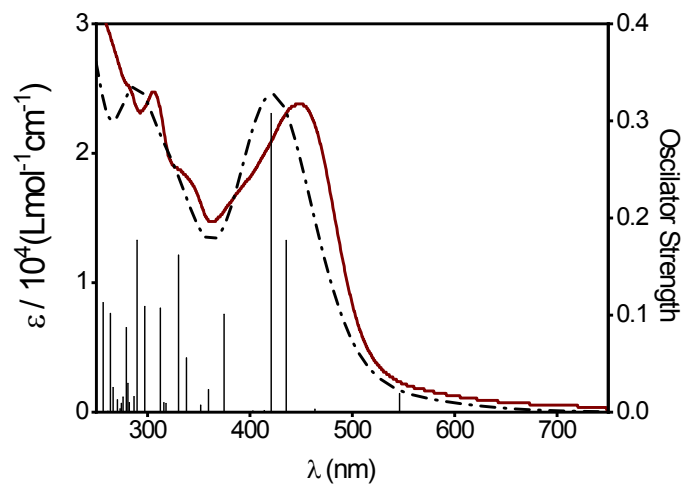


Figure S9. Absorption (—) and emission spectra (----) of *fac*-[ReCl(CO)₃(phen)] (A, $\lambda_{\text{exc}} = 365$ nm), free ligand phet (B, $\lambda_{\text{exc}} = 400$ nm) and *fac*-[ReCl(CO)₃(phet)] (C, $\lambda_{\text{exc}} = 400$ nm) in acetonitrile solution at 298 K.

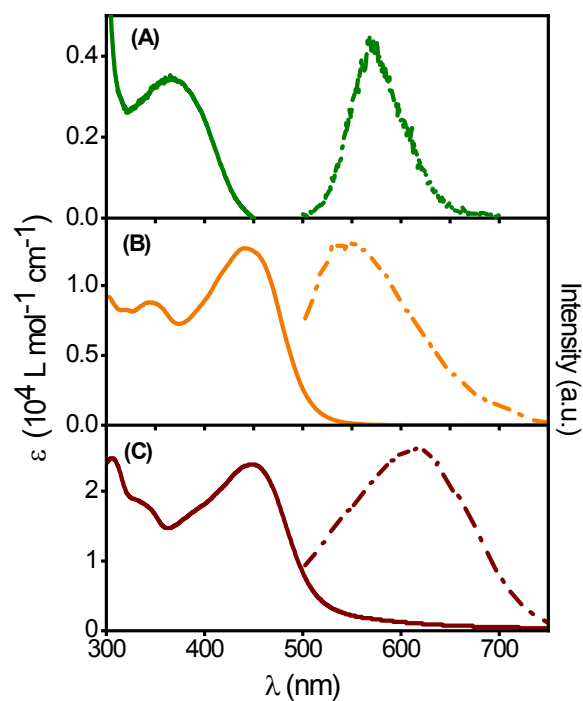


Figure S10. Emission spectra of *fac*-[ReCl(CO)₃(phet)] $\lambda_{\text{exc}} = 400$ nm in acetonitrile saturated with (—) argon or O₂ (—) O₂

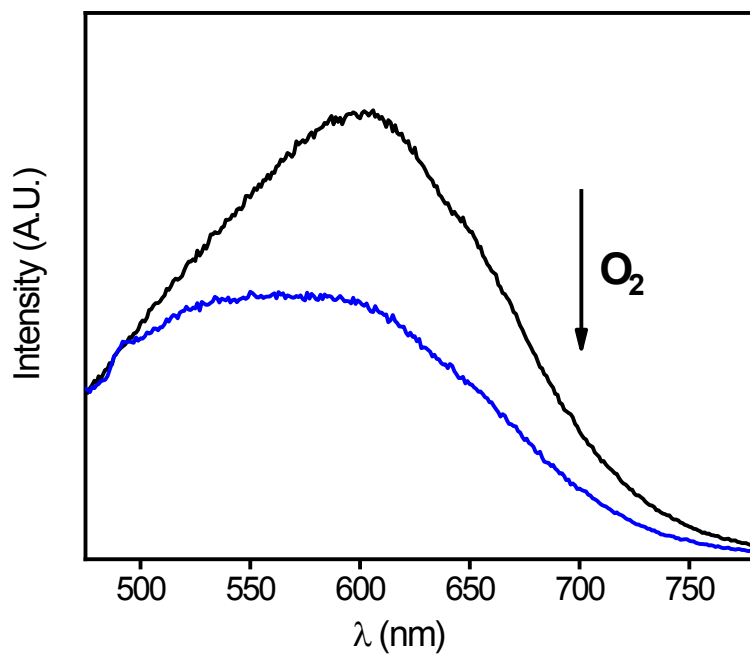


Figure S11. Mono exponential fit (—) of the kinetic traces (○) of the bleaching at 2024 cm⁻¹(A) or of the peak decay at 2024 cm⁻¹ (B).

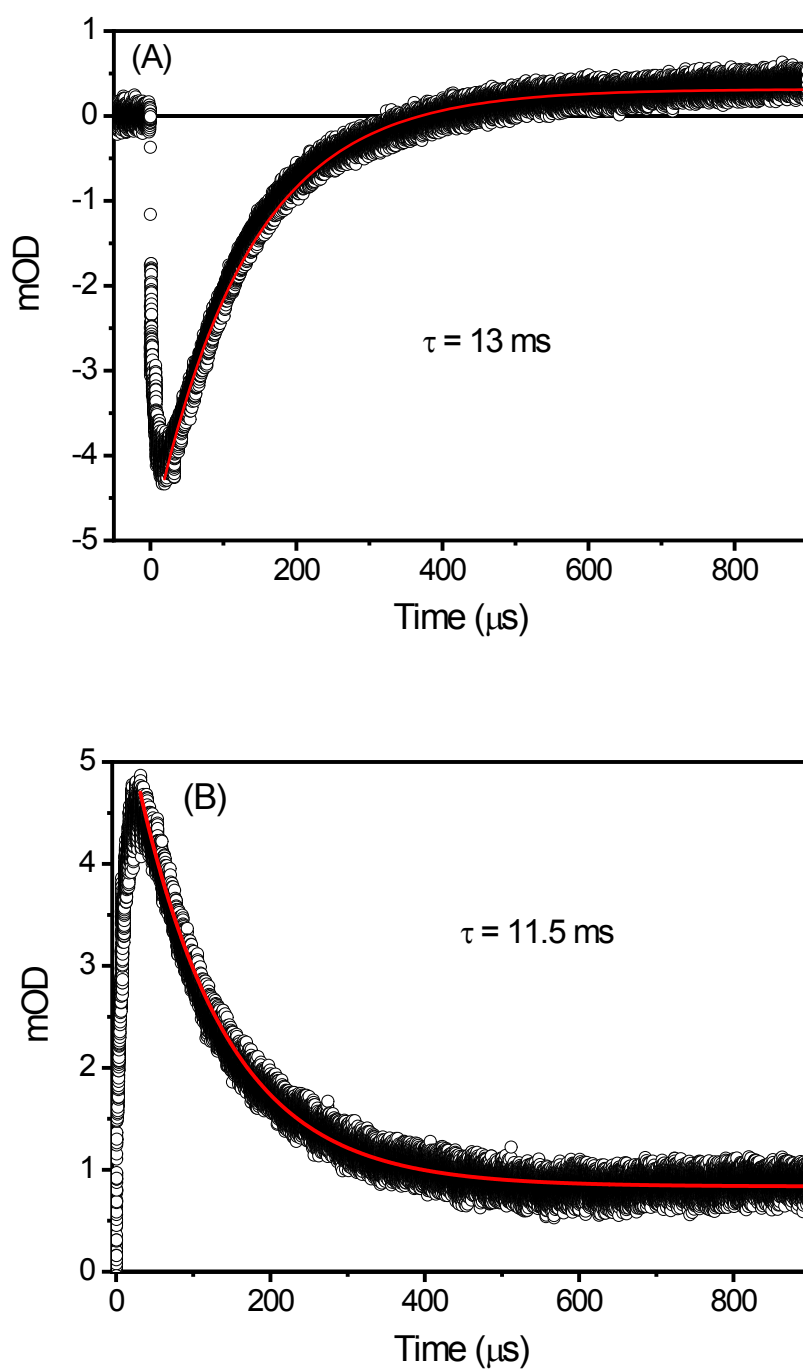


Figure S12. Stacked ^1H -NMR spectra of 0.01 M *fac*-[ReCl(CO) $_3$ (phet)] upon addition of OH $^-$ in DMSO- d_6 –5% water at 298 K. Numbers on the left correspond to the equivalence of anions added.

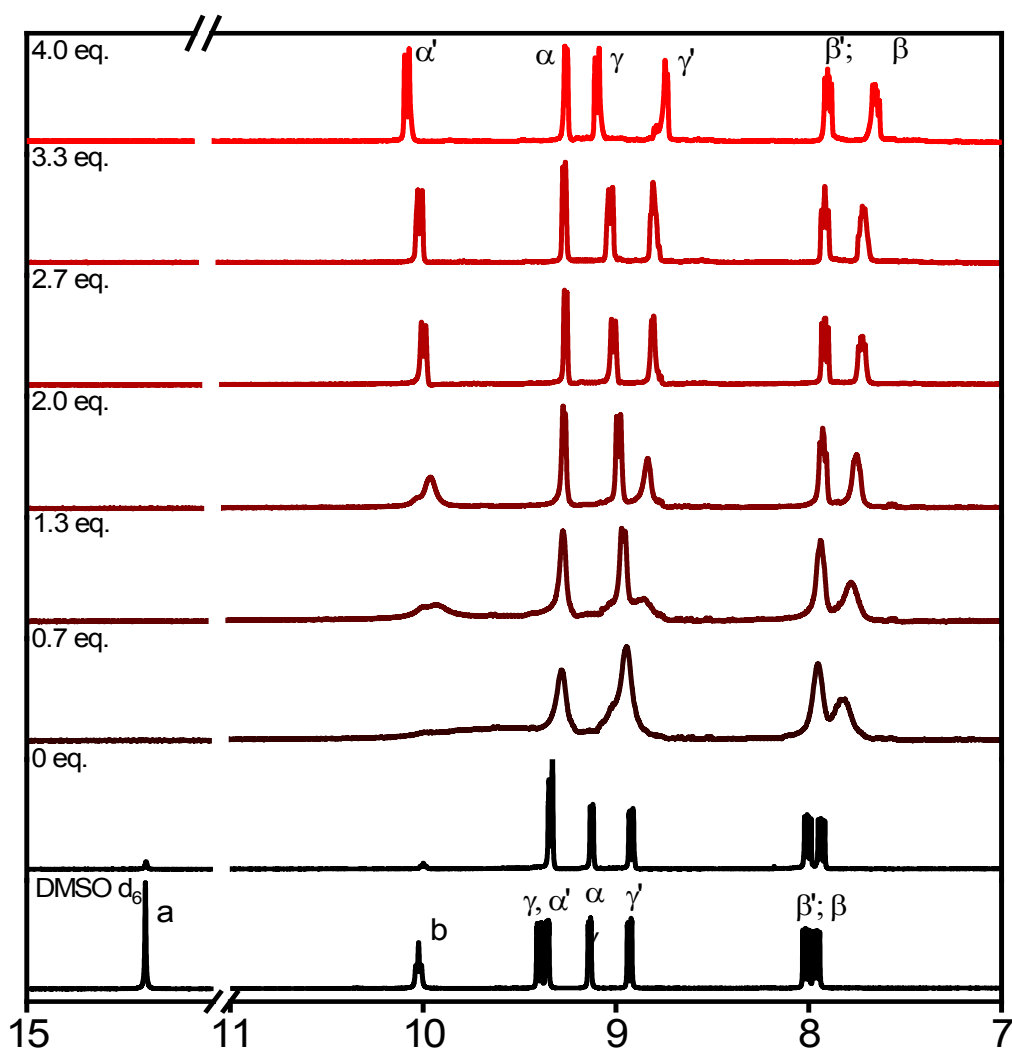


Figure S13. (A) Spectrophotometric titration data monitored at (—) $\lambda_{\text{basic}} = 480$ nm and (—) $\lambda_{\text{acid}} = 445$ nm wavelengths. (B)

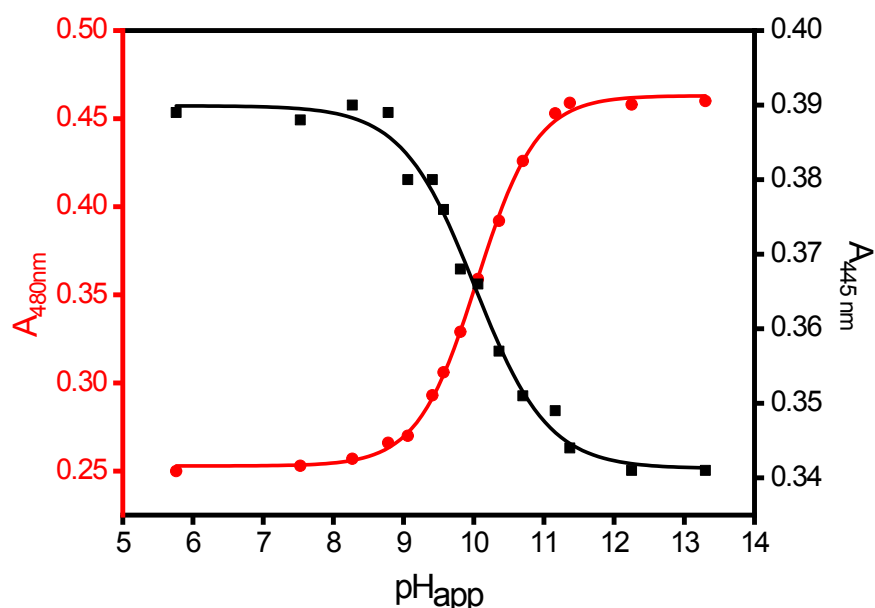


Table S1. Deprotonation thermodynamic parameters of *fac*-[ReCl(CO)₃(phet)], T = 298,15 K.

Deprotonation	$\Delta G_R / \text{KJ mol}^{-1}$	ΔH_R	$T\Delta S_R$
H _a	-13.89	-23.14	-9.25
H _b	-5.03	-7.51	-2.48

Figure S14. Titration Zn²⁺ with *fac*-[ReCl(CO)₃(phet)]

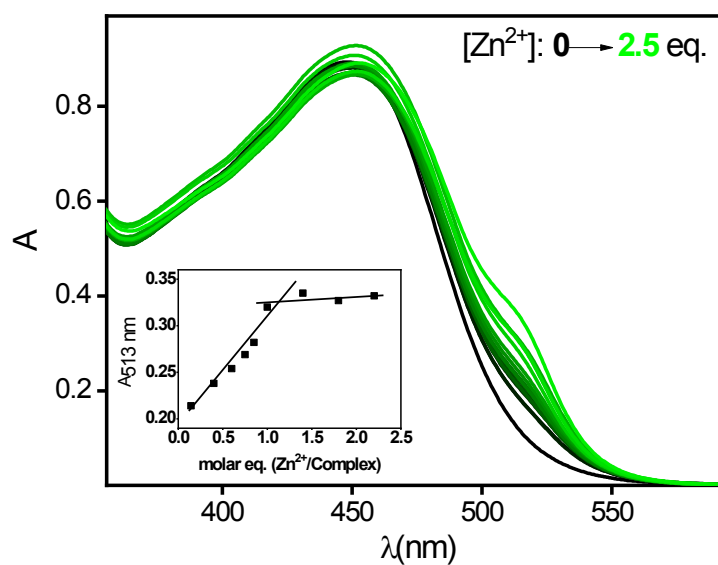


Figure S15. Cyclic Voltammetry of *fac*-[ReCl(CO)₃(phdo)] (red) and *fac*-[ReCl(CO)₃(phet)] (blue); 0,1 mol.L⁻¹ de TBAPF₆ support electrolyte in carbonate propylene. The dashed lines correspond to the blank.

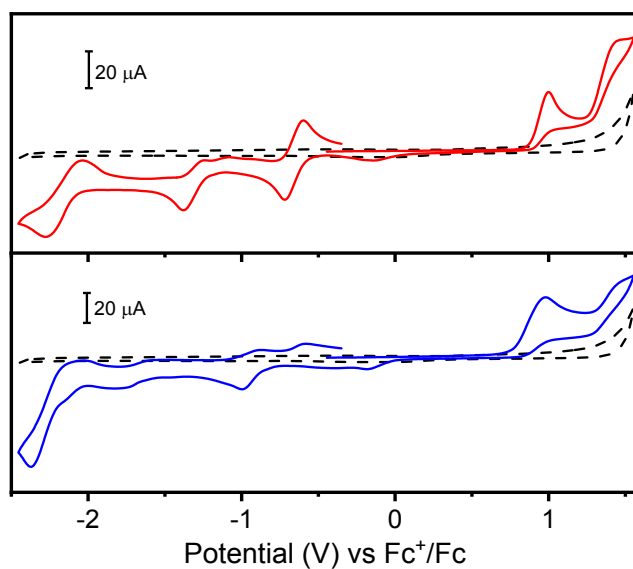


Figure S16. Isosurface plot of the most stable single-occupied molecular orbital of the *fac*-[ReCl(CO)₃(phet)]^{•+} radical

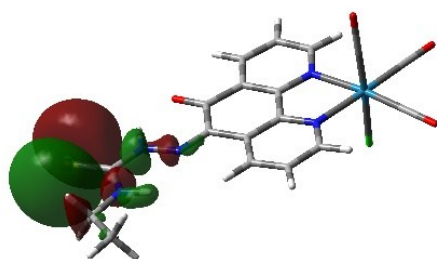


Figure S17. Cyclic voltammetries at different scan rates of the Fc^+/Fc redox pair in CH_3CN (A), free phet in propylene carbonate (B) or of $\text{fac-}[\text{ReCl}(\text{CO})_3(\text{phet})]$ in CH_3CN (C). In (D) it is shown the dependence of the peak current on the square root of the scan rate for the complex $\text{fac-}[\text{ReCl}(\text{CO})_3(\text{phet})]$.

