Electronic Supplementary Material (ESI) for Dalton Transactions.

An Unprecedented One-Step Synthesis of Octahedral Cu(II)-Bis(iminoquinone) Complexes and their Reactivity with $NaBH_4$

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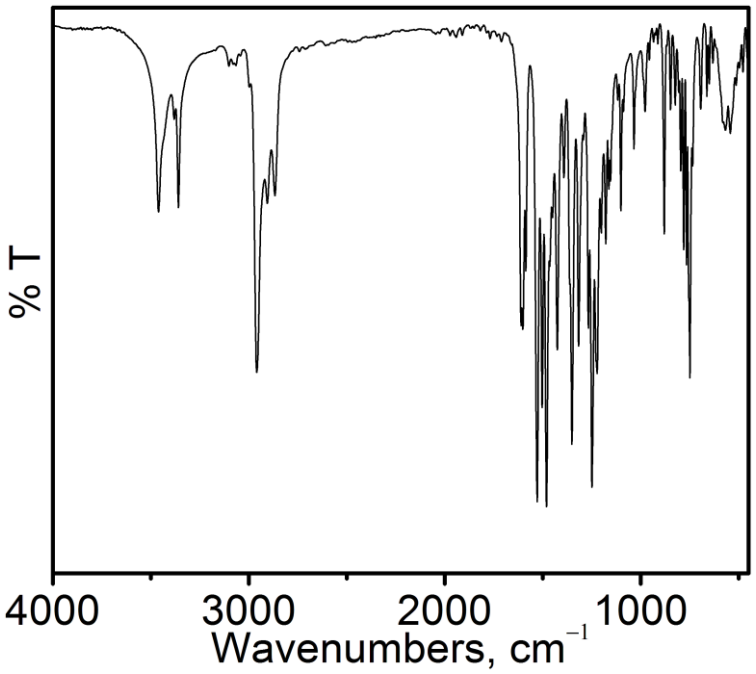


Figure S1: *FTIR spectrum of the ligand,* $\boldsymbol{H_2L^{AP(o\text{–}NO_2\text{–}OPh)}}$.

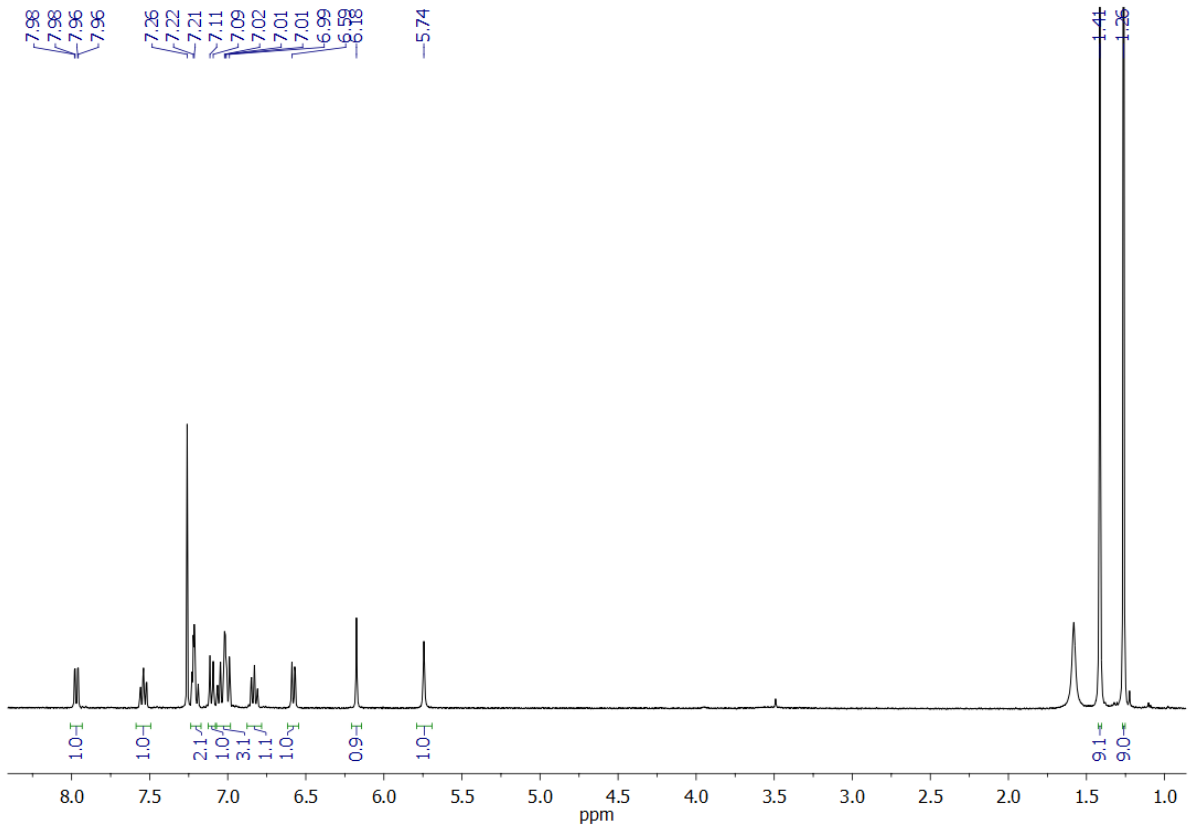


Figure S2: *^{1}H NMR spectrum of the ligand,* $\boldsymbol{H_2L^{AP(o\text{–}NO_2\text{–}OPh)}}$.

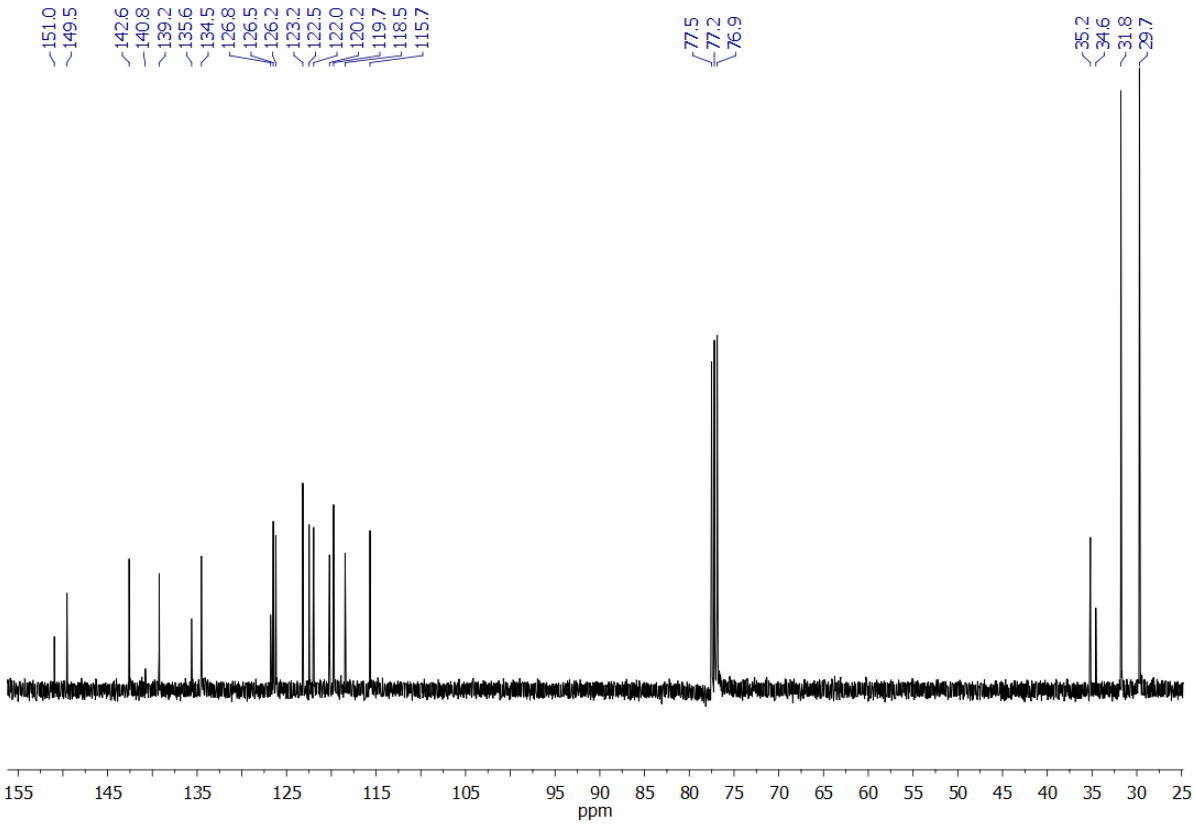


Figure S3: *^{13}C NMR spectrum of the ligand,* $\boldsymbol{H_2L^{AP(o-NO_2-OPh)}}$.

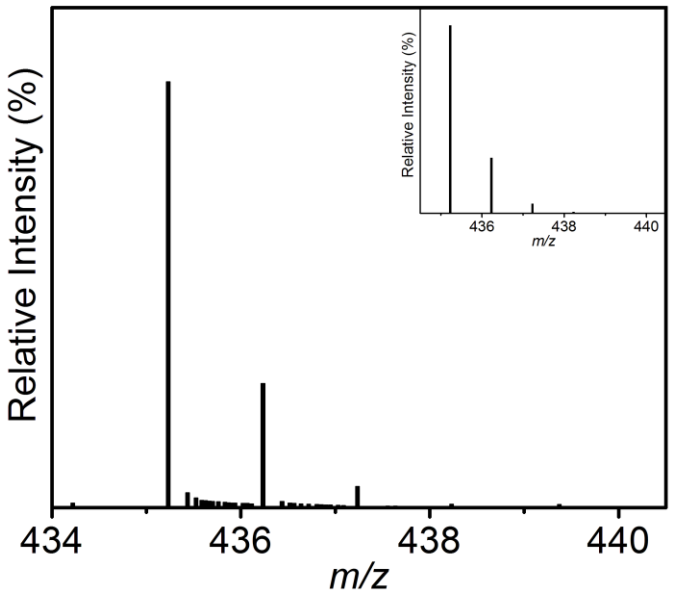


Figure S4: *ESI–mass spectrum for* $\boldsymbol{H_2L^{AP(o-NO_2-OPh)}}$ *in +ve mode; experimental and simulated isotopic distribution pattern (inset).*

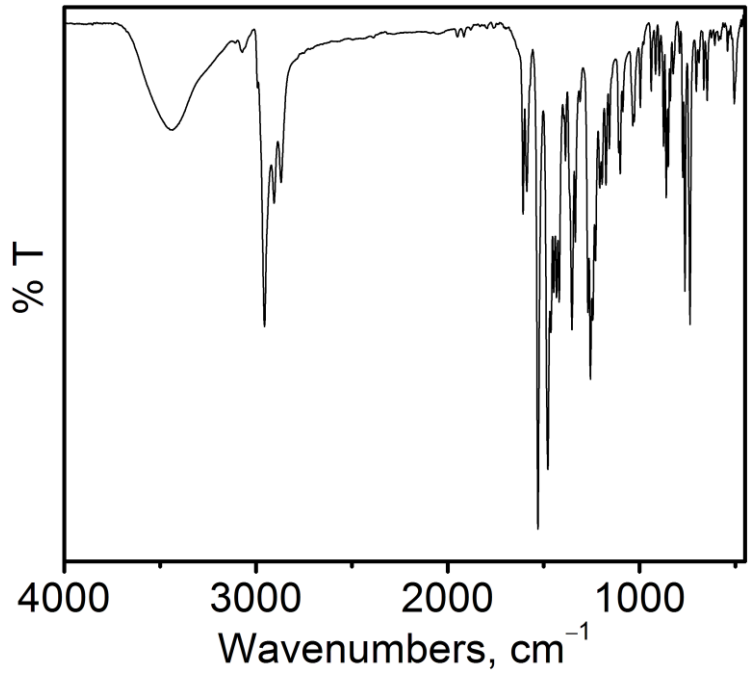


Figure S5: *FTIR spectrum of complex **1**.*

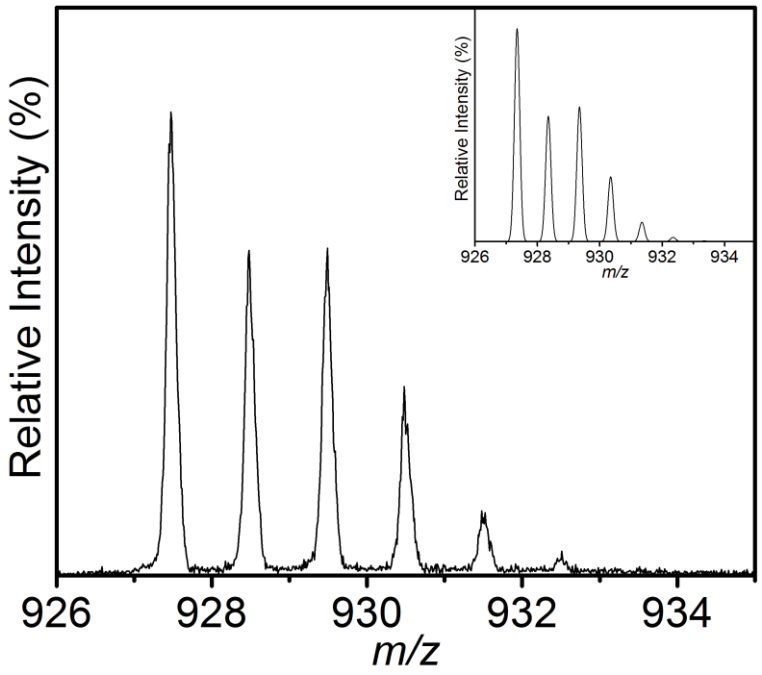


Figure S6: *ESI–mass spectrum for **1** in +ve mode; experimental and simulated isotopic distribution pattern (inset).*

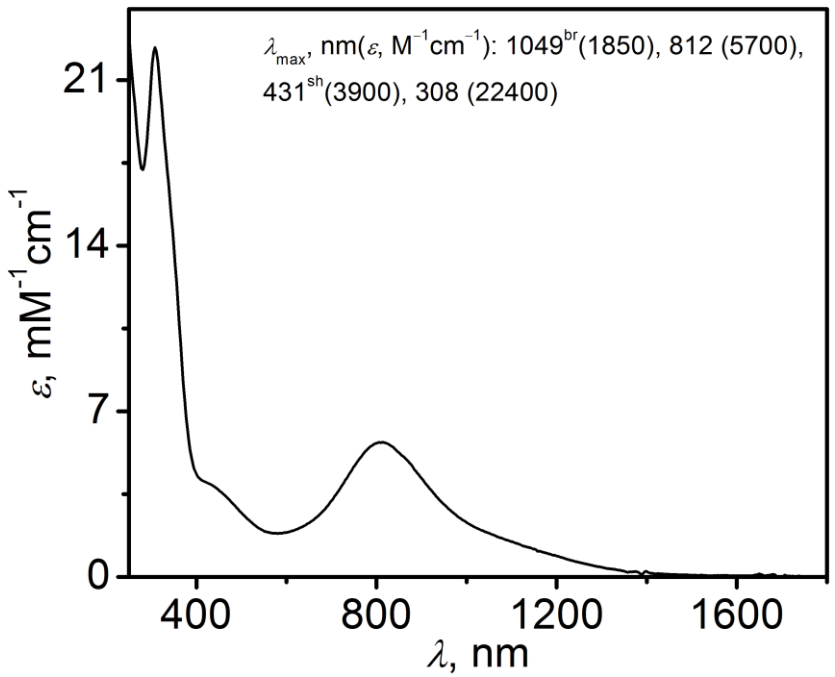


Figure S7: *UV–vis/NIR spectrum of **1** measured at room temperature (RT) in dichloromethane solution in 250–1600 nm range.*

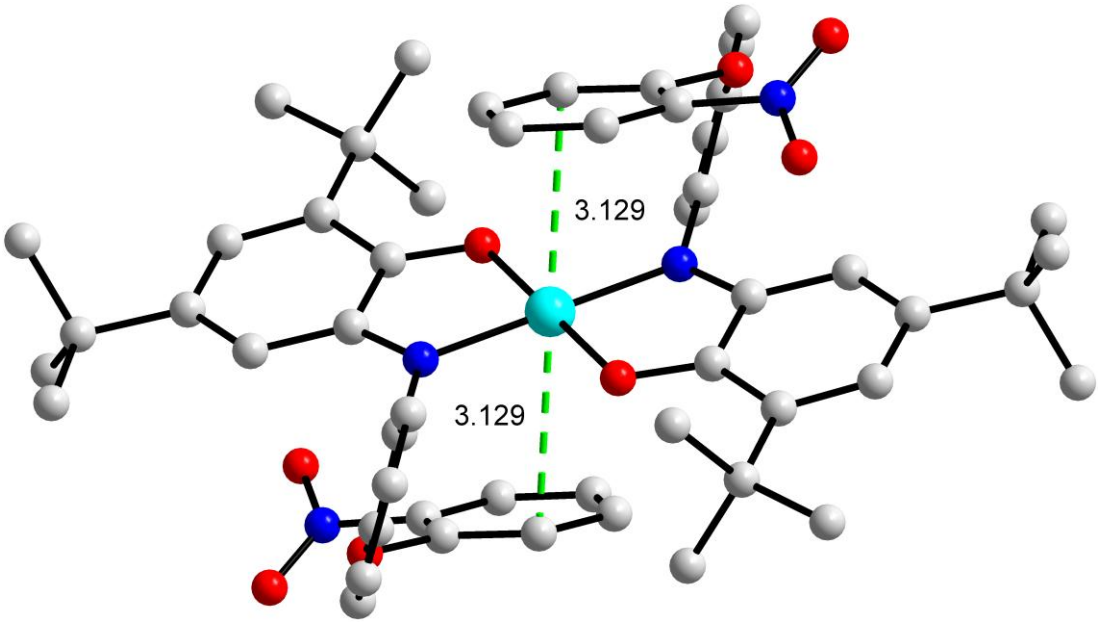


Figure S8: *Showing Cu(II)-C_{Ph} interaction in complex **1**. grey = C, red = O, blue = N, cyan = Cu. Distance is in Å.*

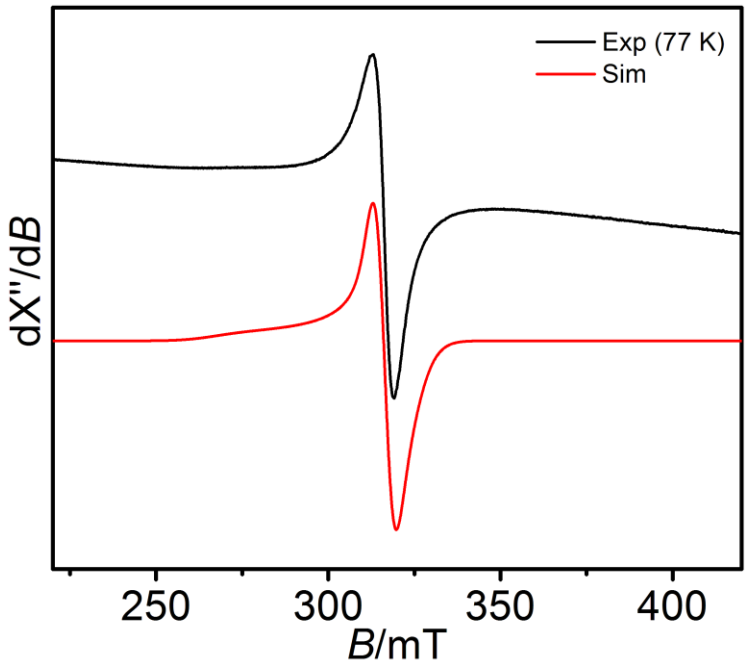


Figure S9: *Experimental X–band EPR spectra for complexes **1** in solid state at 77 K; X-band microwave frequency (GHz): 9.145, modulation frequency (kHz): 100, microwave power (mW): 0.998, amplitude: 1.0.*

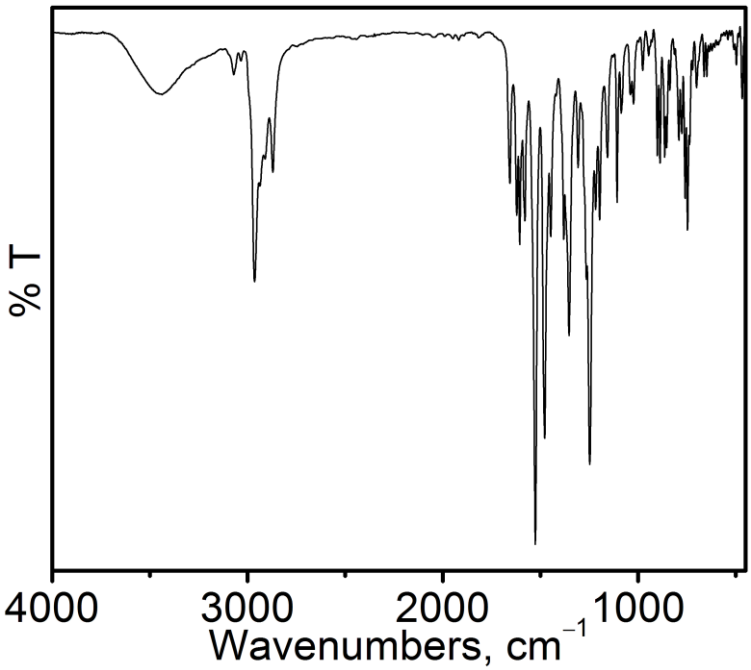


Figure S10: *FTIR spectrum of complex **2**.*

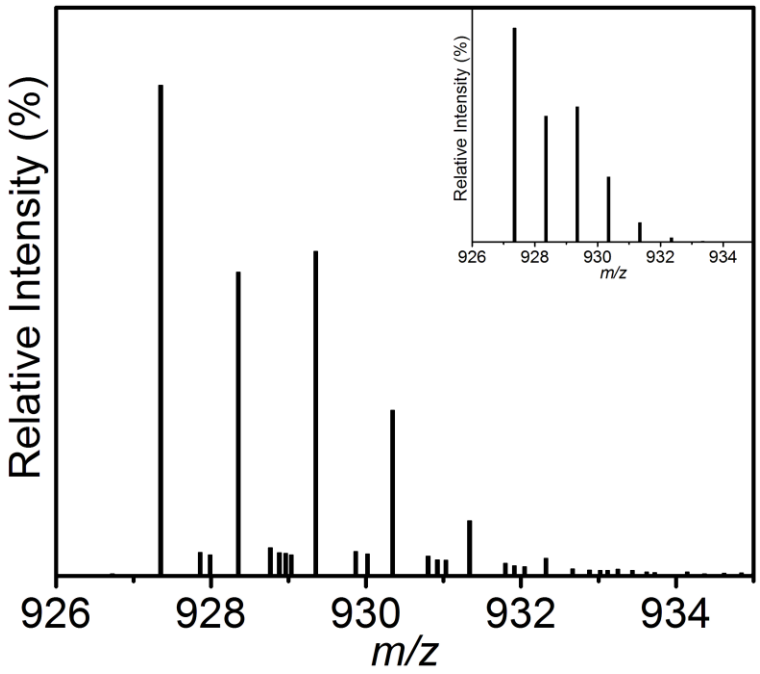


Figure S11: *ESI–mass spectrum for **2** in +ve mode; experimental and simulated isotopic distribution pattern (inset).*

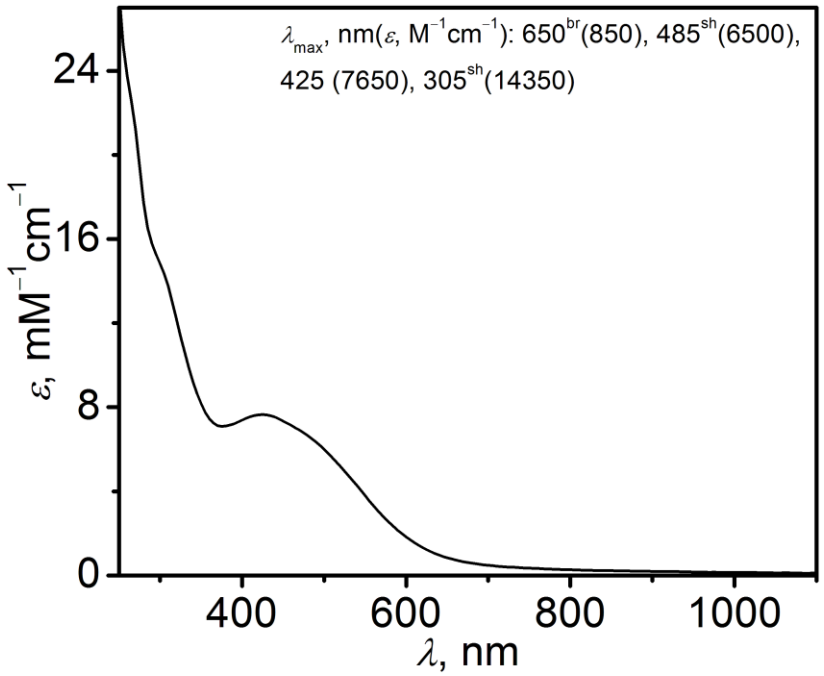


Figure S12: *UV–vis/NIR spectrum of **2** measured at room temperature (RT) in dichloromethane solution in 250–1100 nm range.*

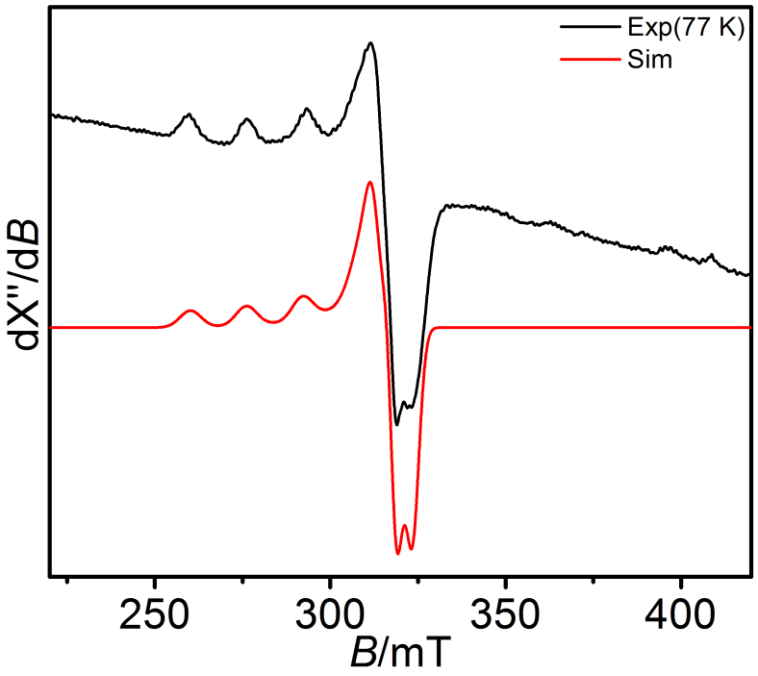


Figure S13: *Experimental X–band EPR spectra for complexes **2** in a 5:1 CH_2Cl_2/Toluene solvent mixture at 77 K; X-band microwave frequency (GHz): 9.143, modulation frequency (kHz): 100, microwave power (mW): 0.995, amplitude: 3.0.*

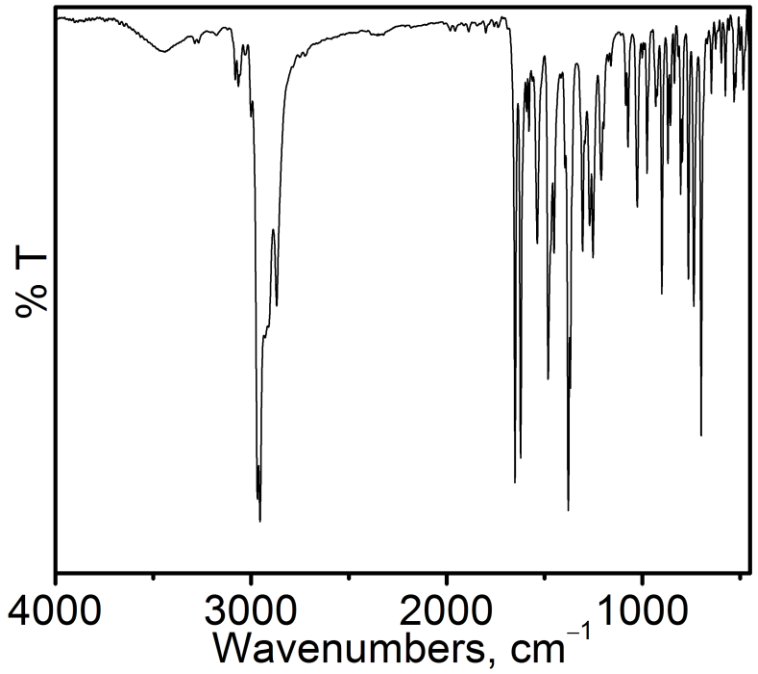


Figure S14: *FTIR spectrum of complex **3**.*

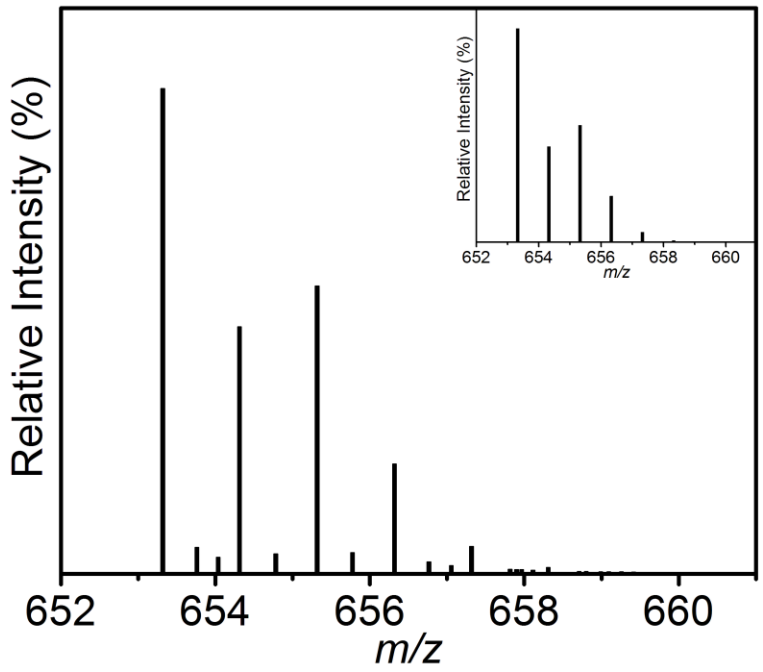


Figure S15: *ESI–mass spectrum for **3** in +ve mode; experimental and simulated isotopic distribution pattern (inset).*

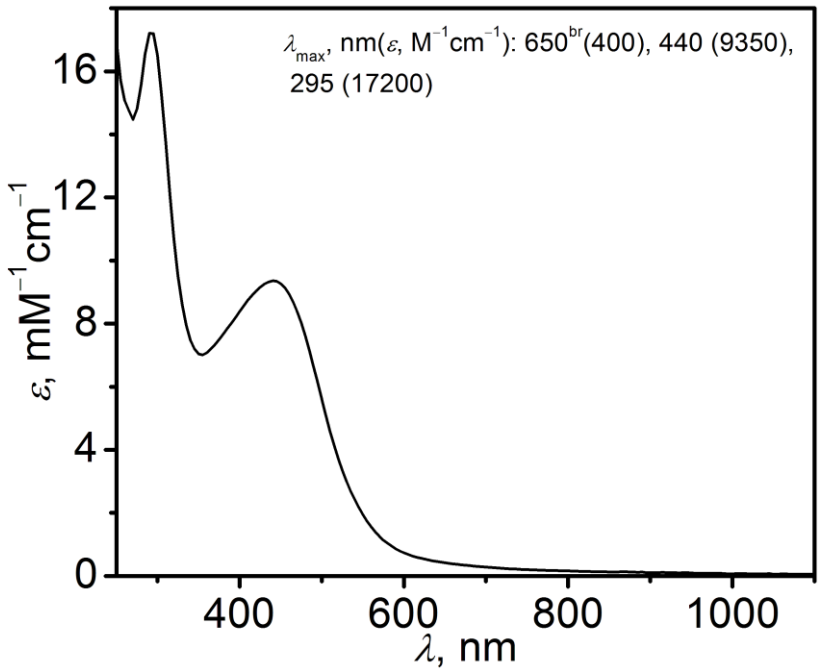


Figure S16: *UV–vis/NIR spectrum of **3** measured at room temperature (RT) in dichloromethane solution in 250–1100 nm range.*

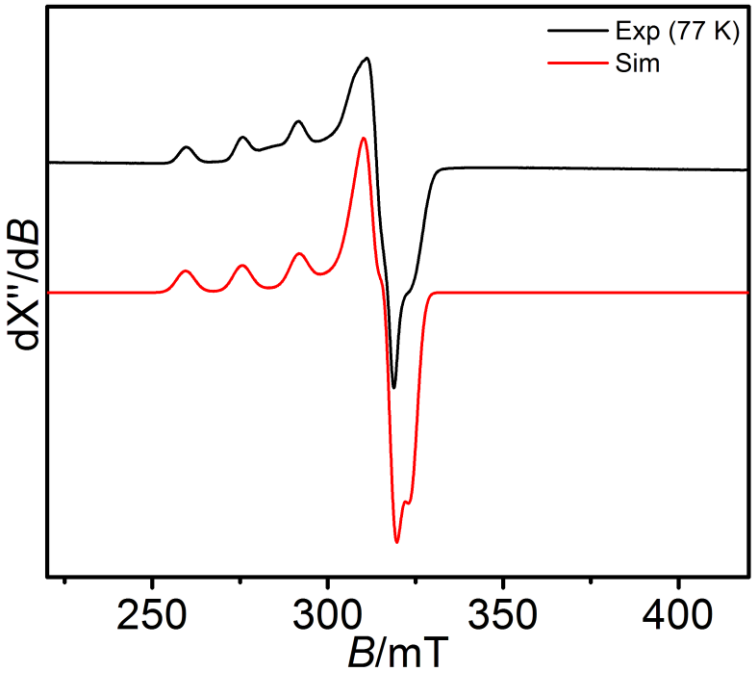


Figure S17: *Experimental X–band EPR spectra for complexes **3** in a 5:1 CH_2Cl_2/Toluene solvent mixture at 77 K; X-band microwave frequency (GHz): 9.142, modulation frequency (kHz): 100, microwave power (mW): 0.995, amplitude: 1.0.*

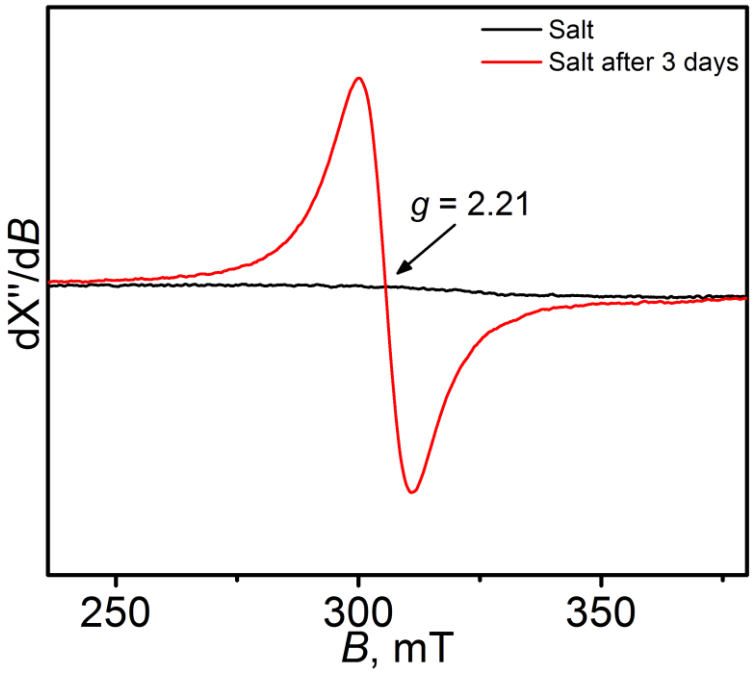
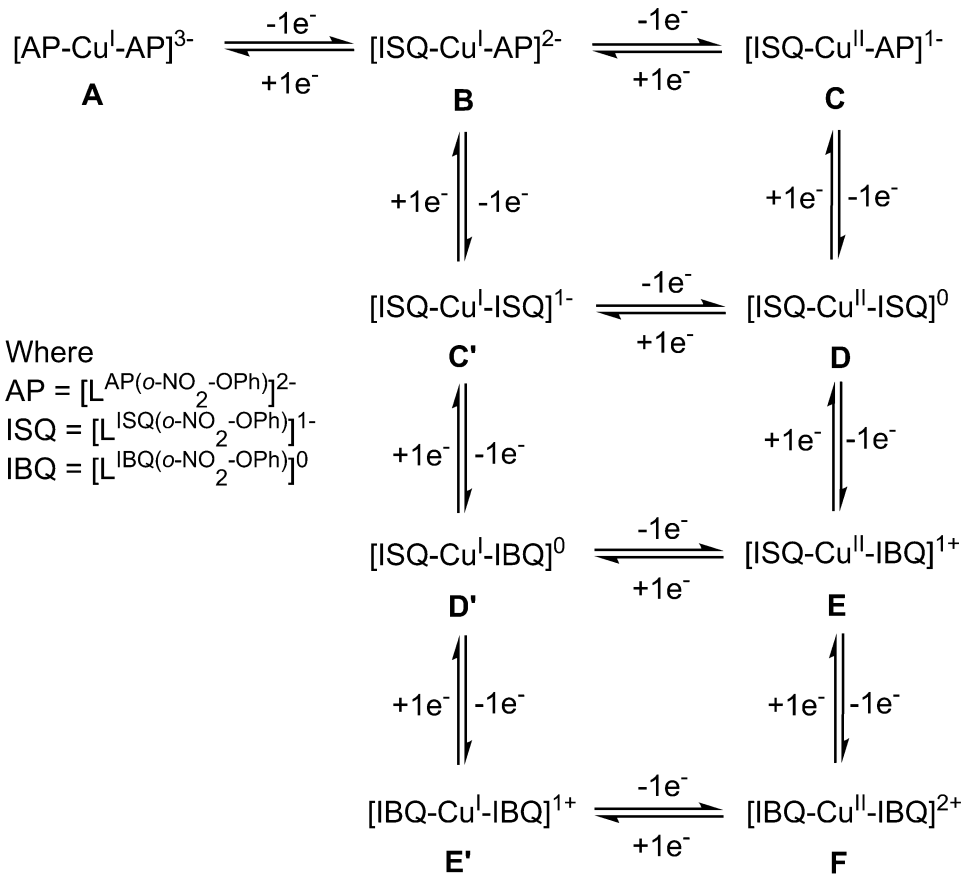


Figure S18: *Experimental X–band EPR spectra for the salt found during the synthesis of complex **2** at room temperature; X-band microwave frequency (GHz): 9.450, modulation frequency (kHz): 100, microwave power (mW): 0.998, amplitude (G): 100.0.*



Scheme 1. Possible redox states of complex **1**.

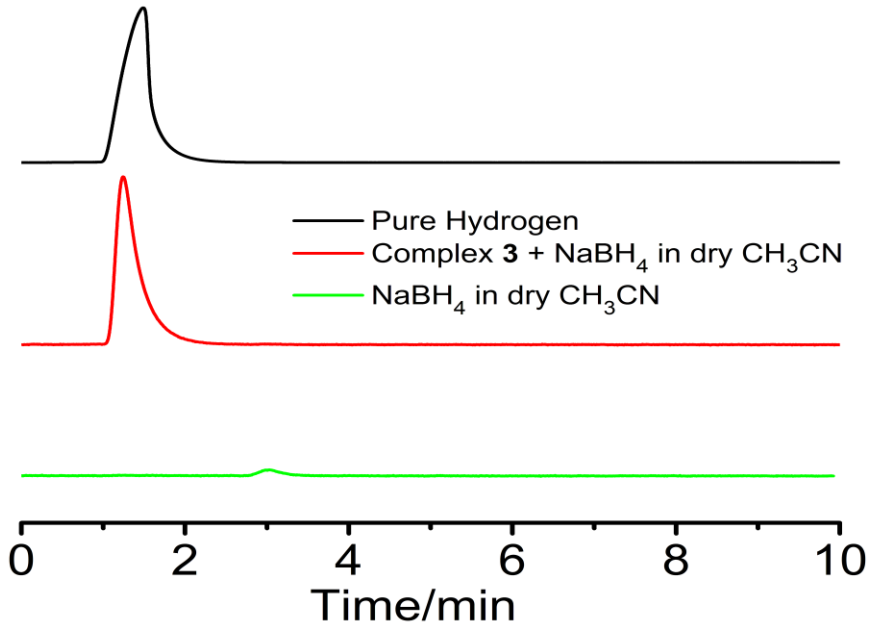


Figure S19: *GC spectra showing the production of H_2 gas in the presence of complex **3** and no production of H_2 gas in absence of the complex in CH_3CN. For all measurements 25 μl gas was used.*

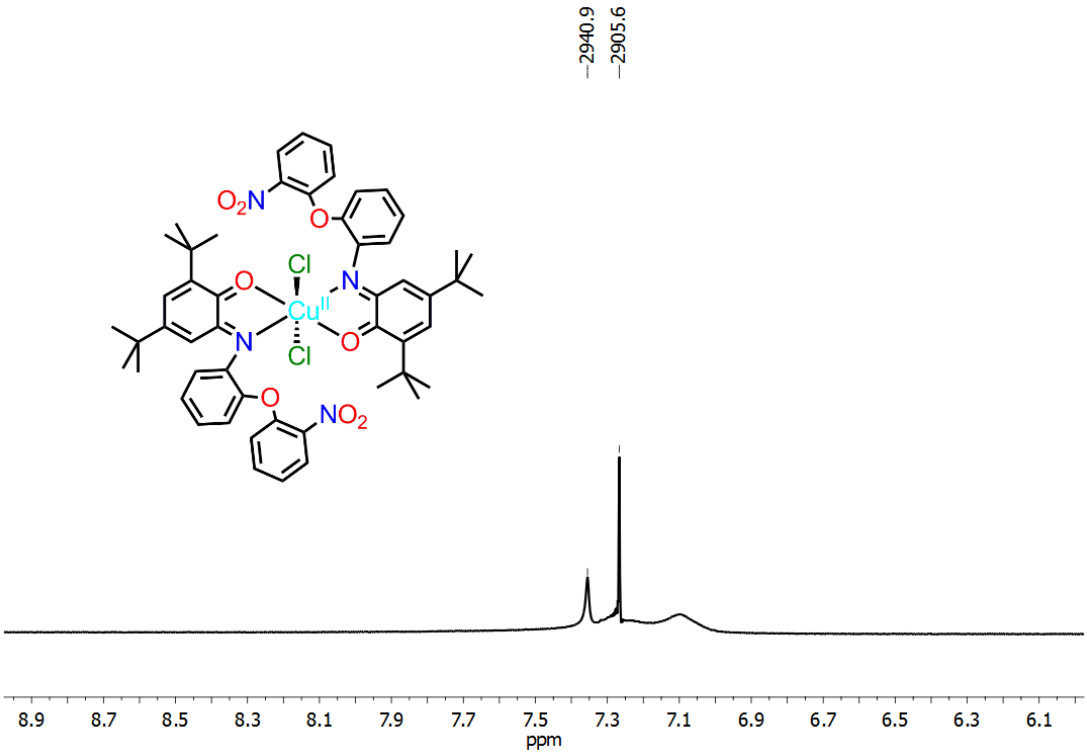


Figure 20: *Evans method ^{1}H NMR spectrum of complex **2** in $CDCl_3$ at 400 MHz. μ_{eff} =2.05 μ_B.*

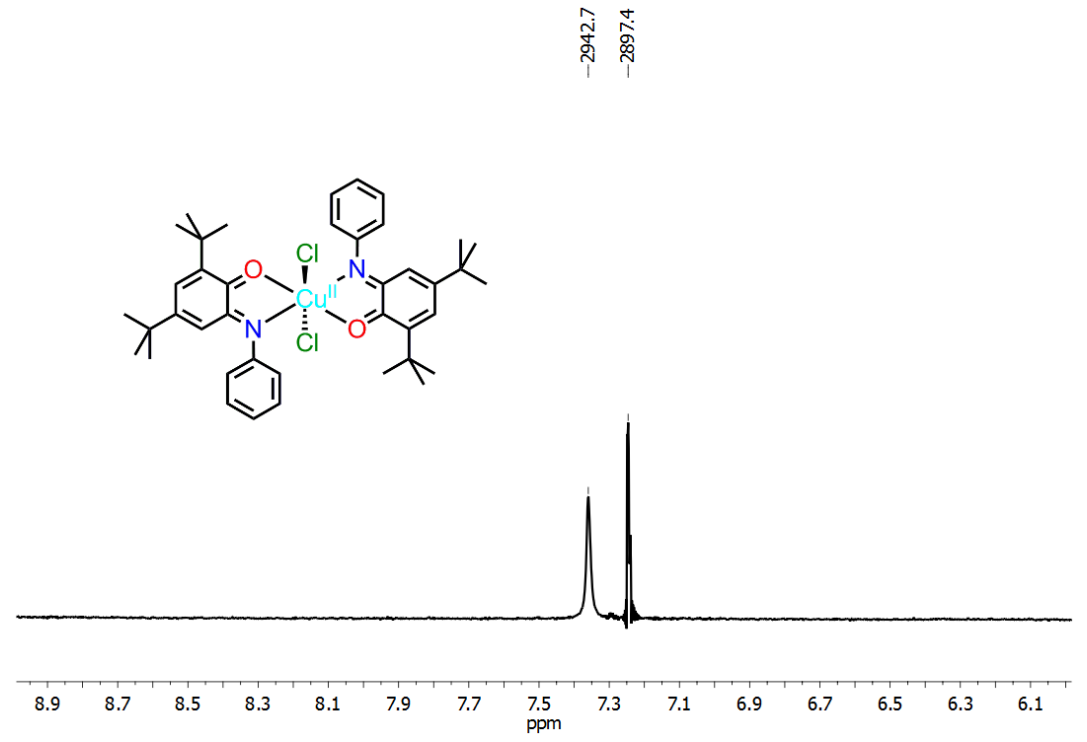


Figure 21: *Evans method ^{1}H NMR spectrum of complex **3**•CH_2Cl_2 in $CDCl_3$ at 400 MHz. μ_{eff} =1.95 μ_B.*