

Supporting Information

Synthesis and Structural Characterization of the Silver(I), Copper(I) Coordination Polymers and the Helicate Palladium(II) Complex of the Dipyrrolylmethane-based Dipyrazole Ligands: The Effect of Meso Substituents on the Structure Formation

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NMR and IR Spectra

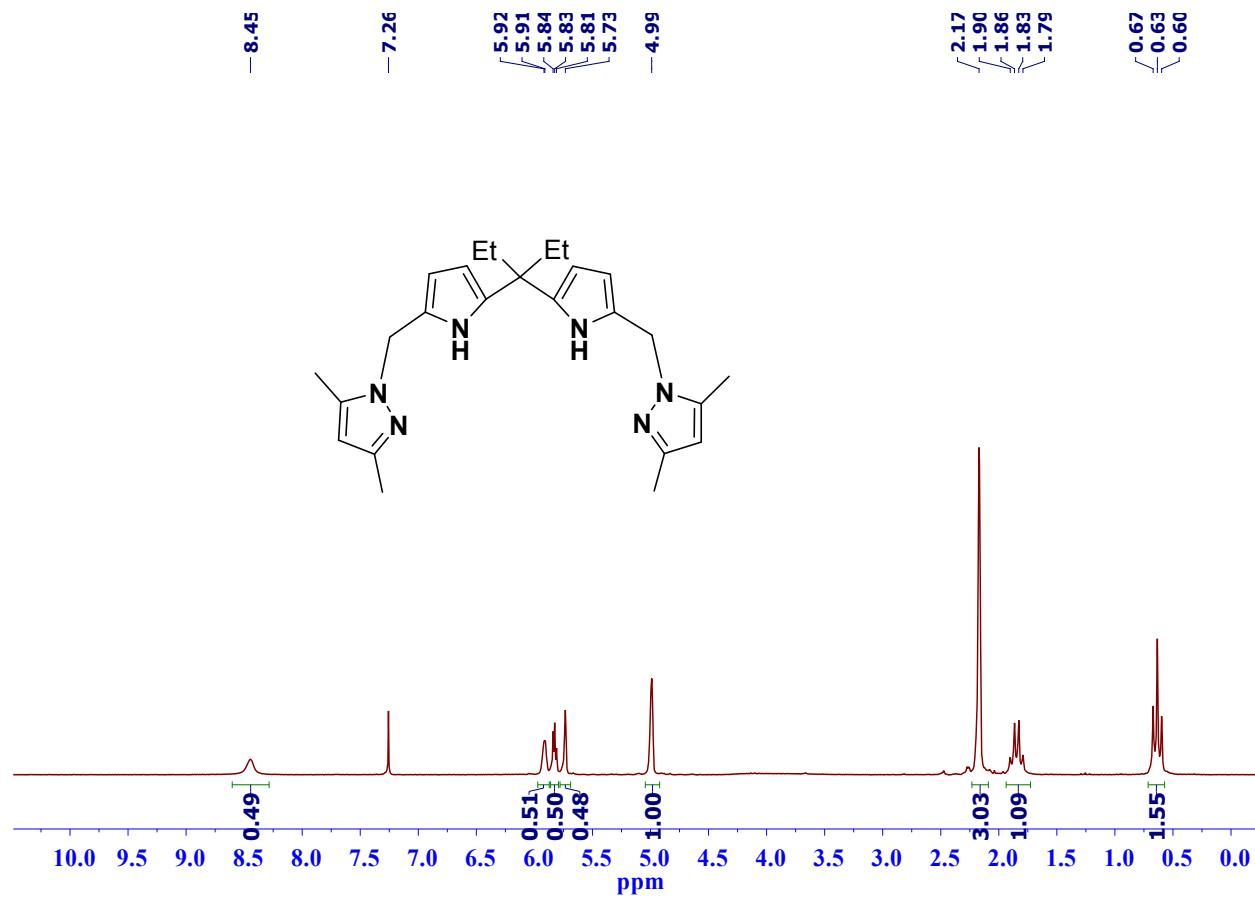


Figure S1: ^1H NMR (200 MHz) spectrum of L_1 in CDCl_3 at room temperature.

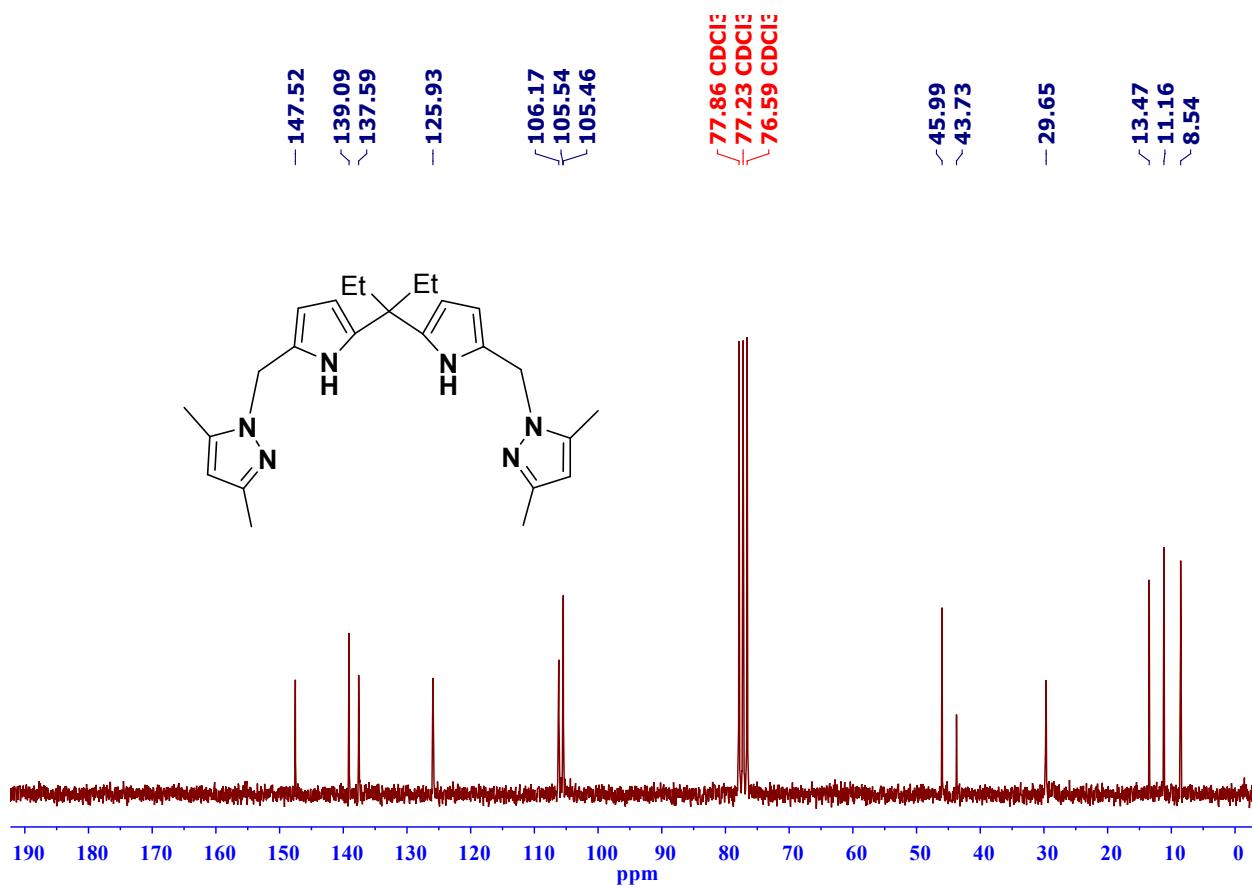


Figure S2: $^{13}\text{C}\{^1\text{H}\}$ NMR (50.3 MHz) spectrum of **L**₁ in CDCl_3 at room temperature.

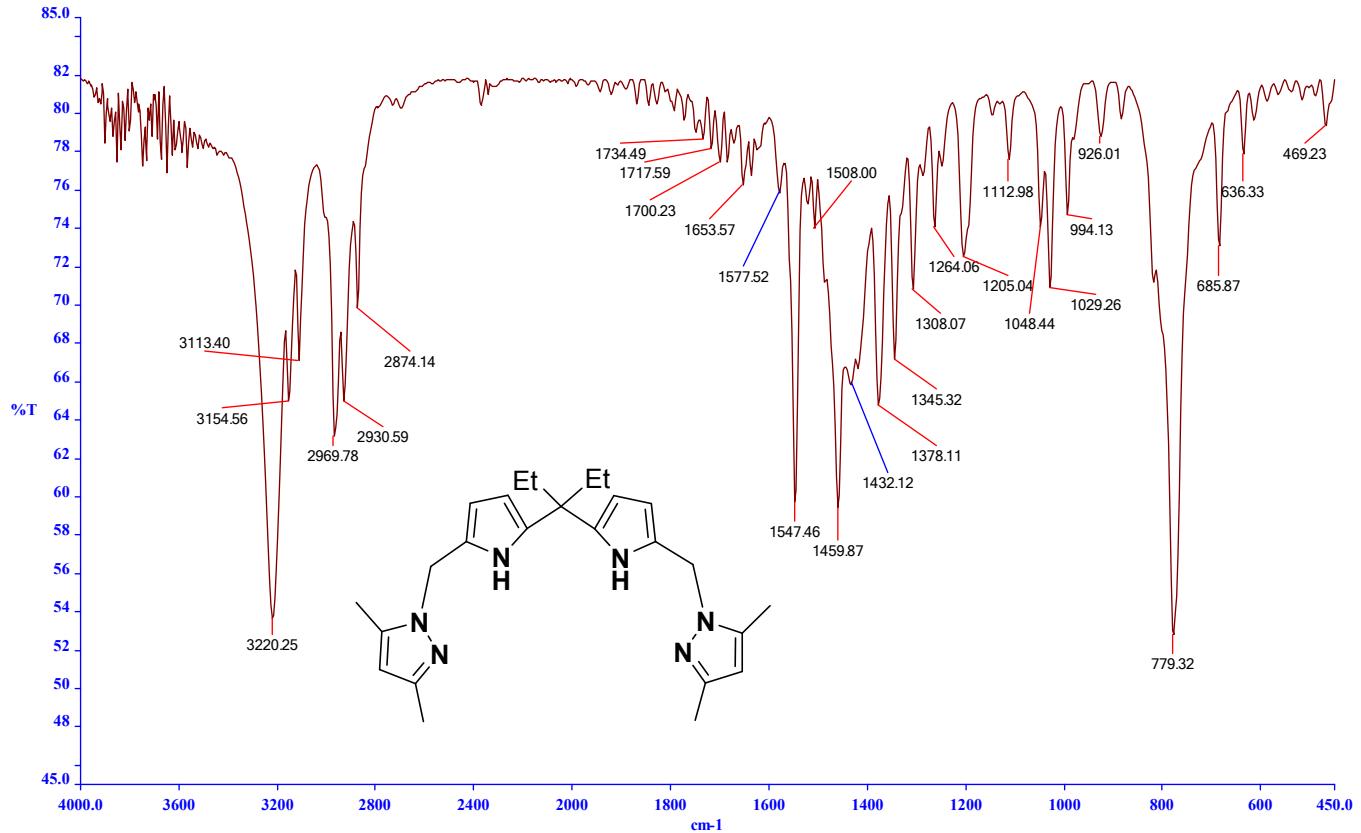


Figure S3: IR spectrum of L_1 recorded as a KBr disc.

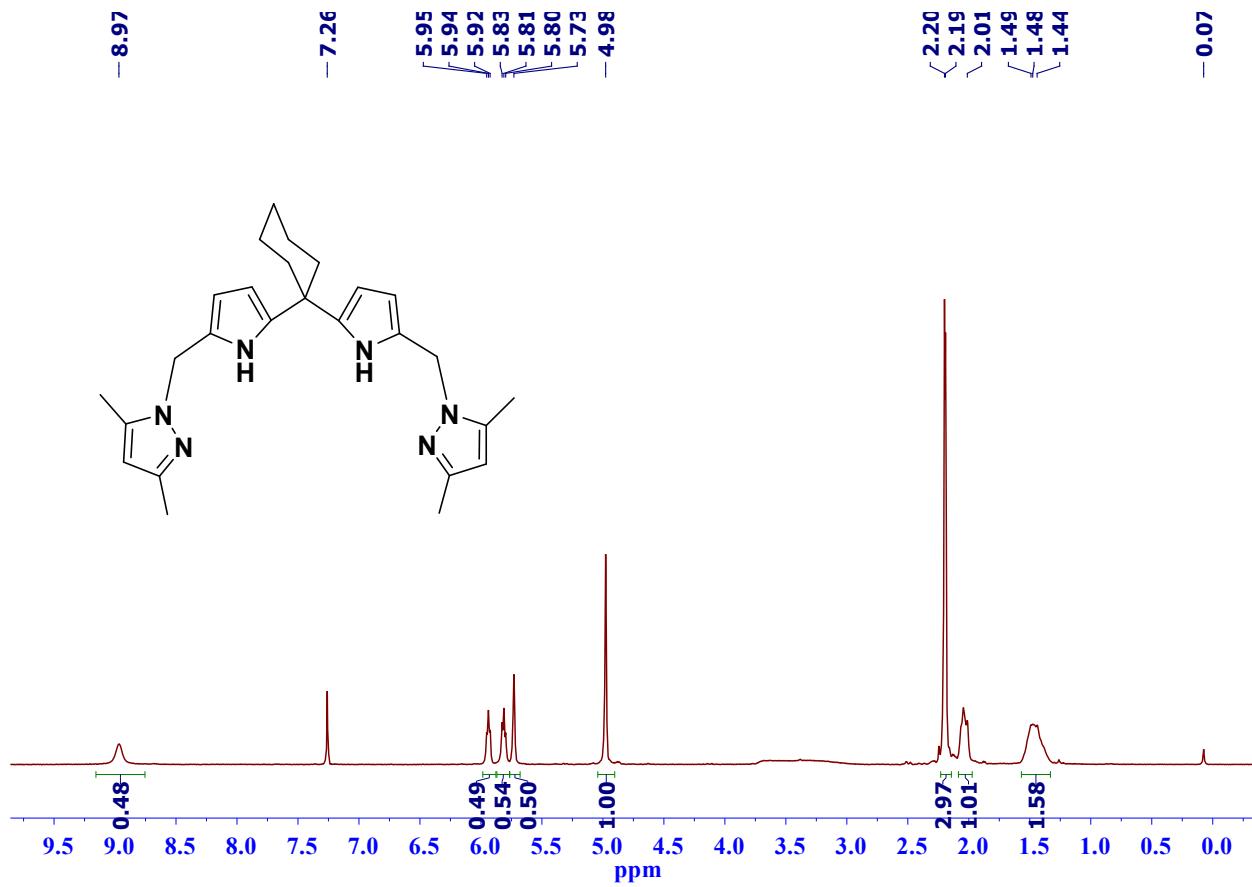


Figure S4: ^1H NMR (200 MHz) spectrum of \mathbf{L}_2 in CDCl_3 at room temperature.

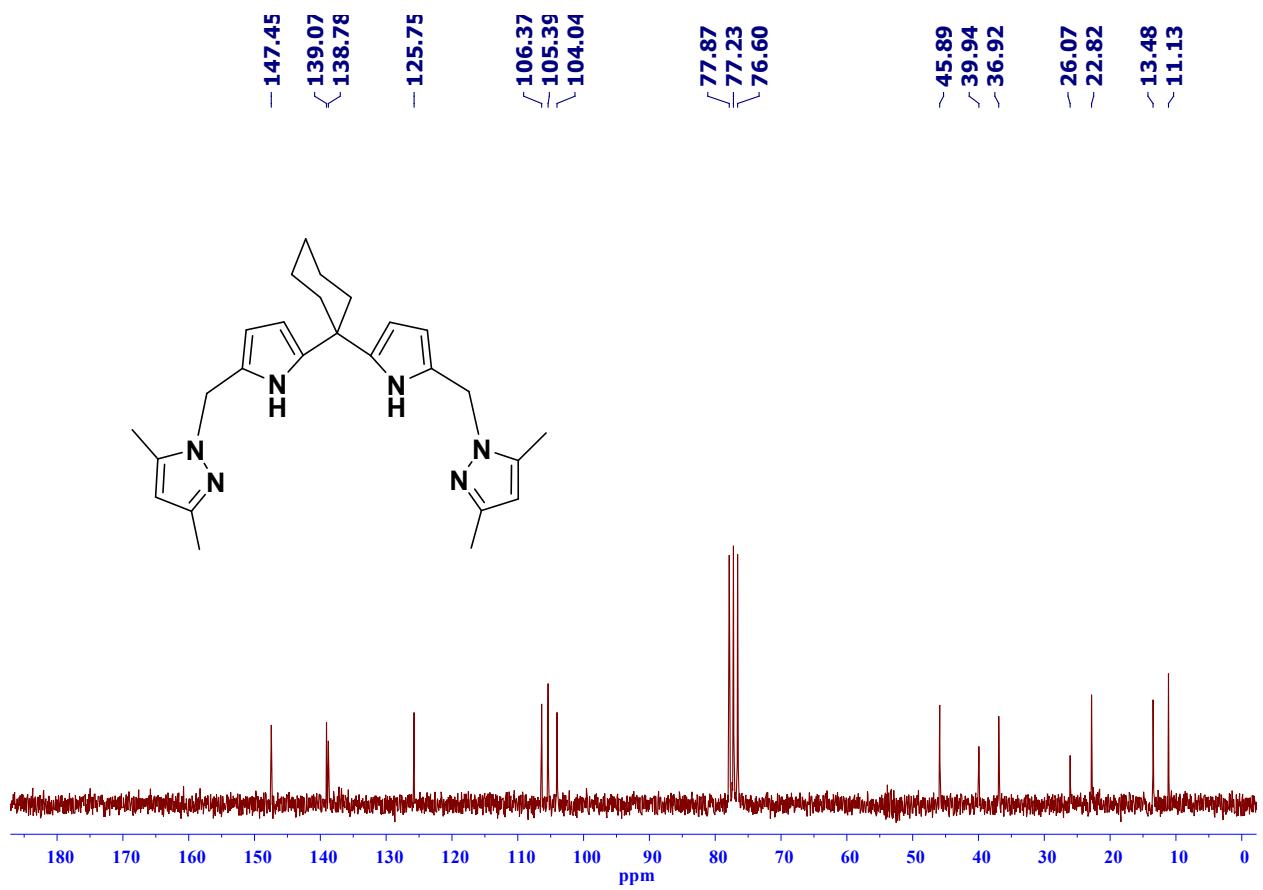


Figure S5: $^{13}\text{C}\{\text{H}\}$ NMR (50.3 MHz) spectrum of \mathbf{L}_2 in CDCl_3 at room temperature.

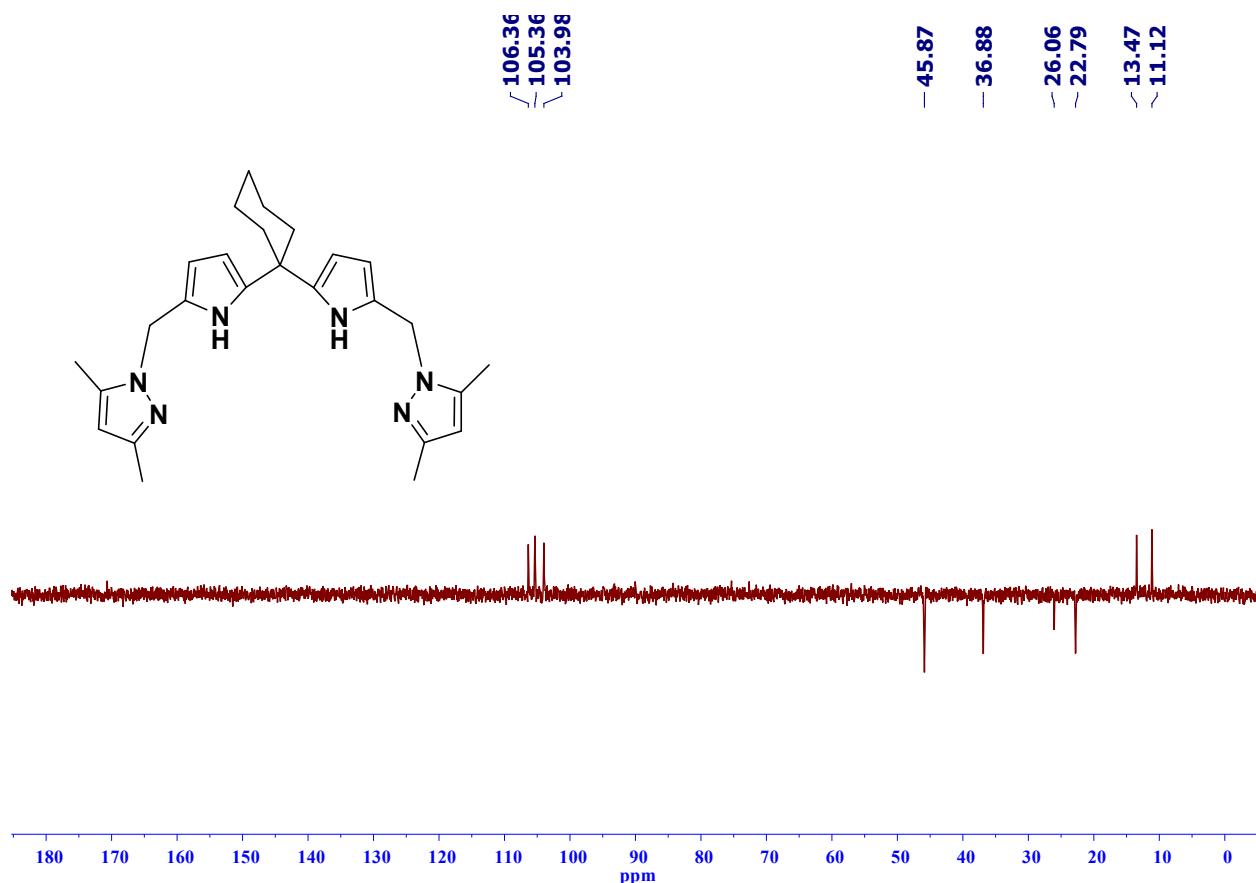


Figure S6: DEPT-135 $\{\text{H}\}$ NMR (50.3 MHz) spectrum of \mathbf{L}_2 in CDCl_3 at room temperature.

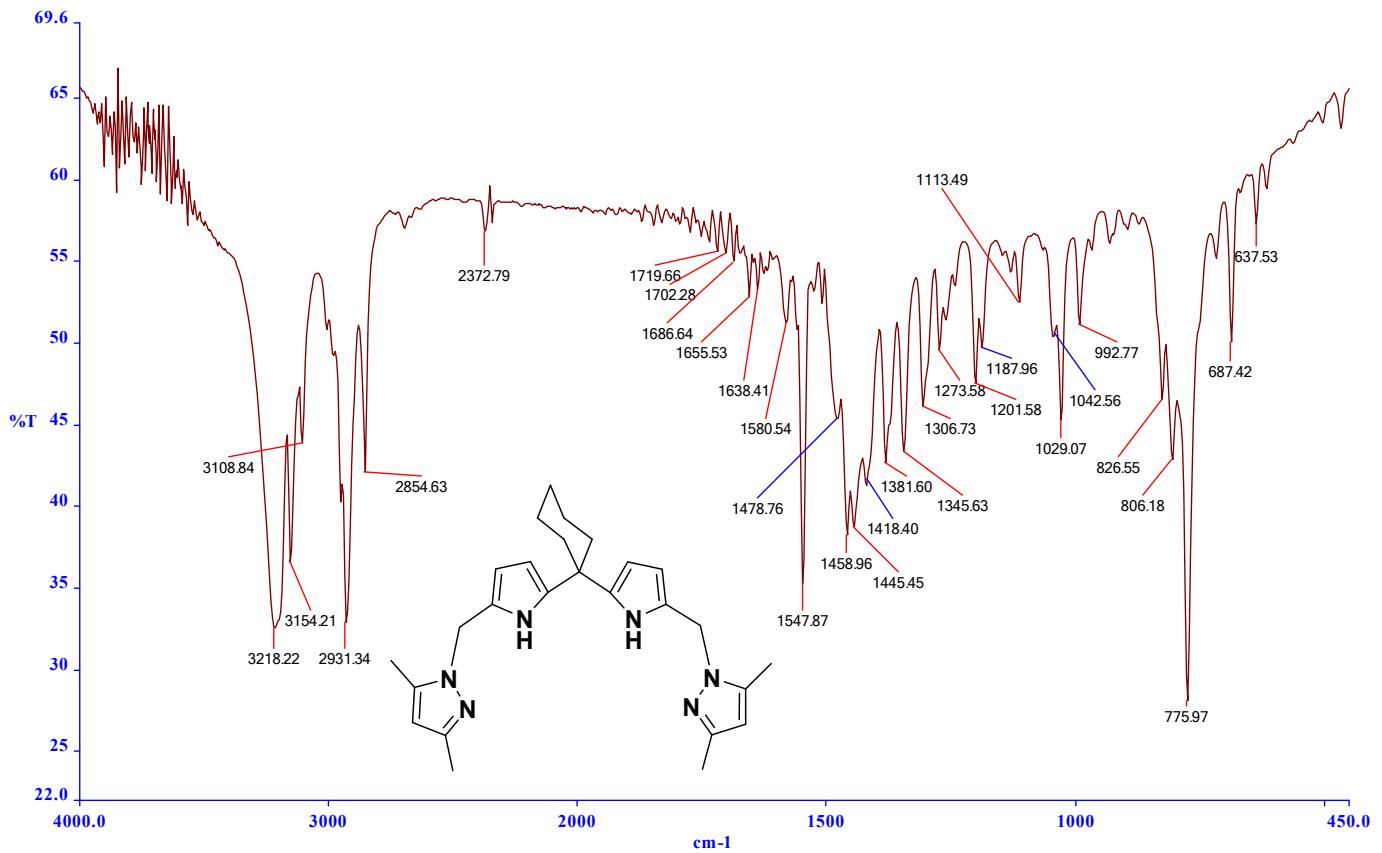


Figure S7: IR spectrum of L_2 recorded as a KBr disc.

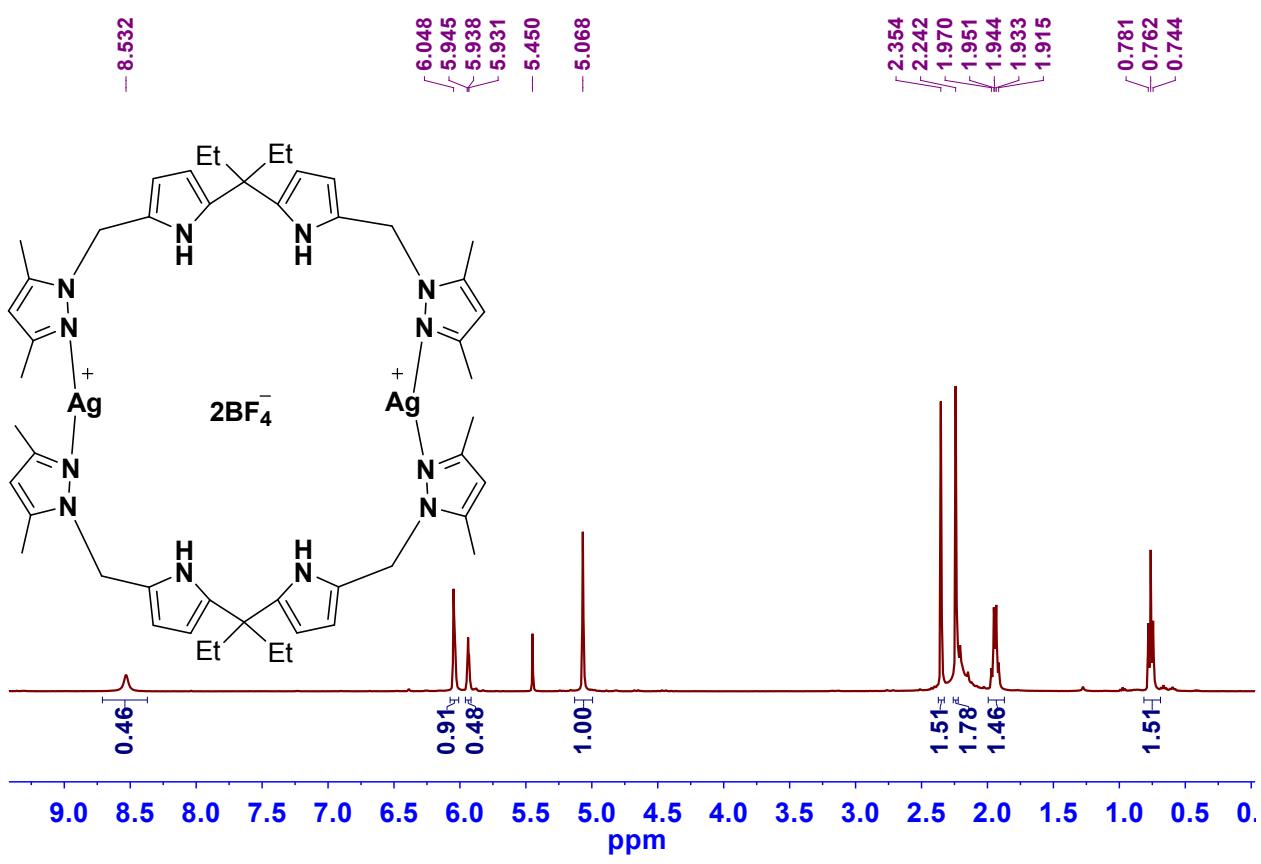


Figure S8: ^1H NMR (400 MHz) spectrum of silver(I) complex 4 in CD_3CN at room temperature.

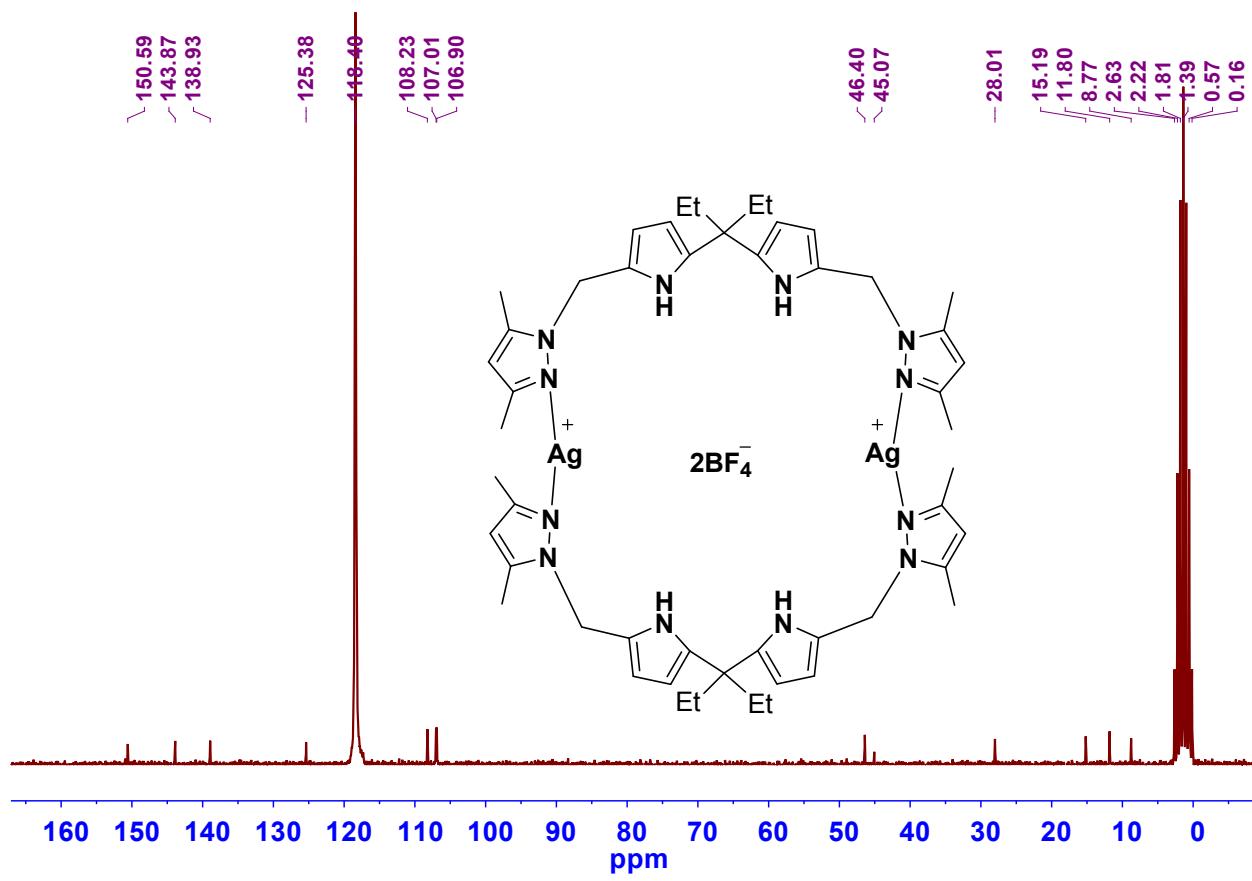


Figure S9: $^{13}\text{C}\{^1\text{H}\}$ NMR (50.3 MHz) spectrum of silver(I) complex **4** in CD_3CN at room temperature.

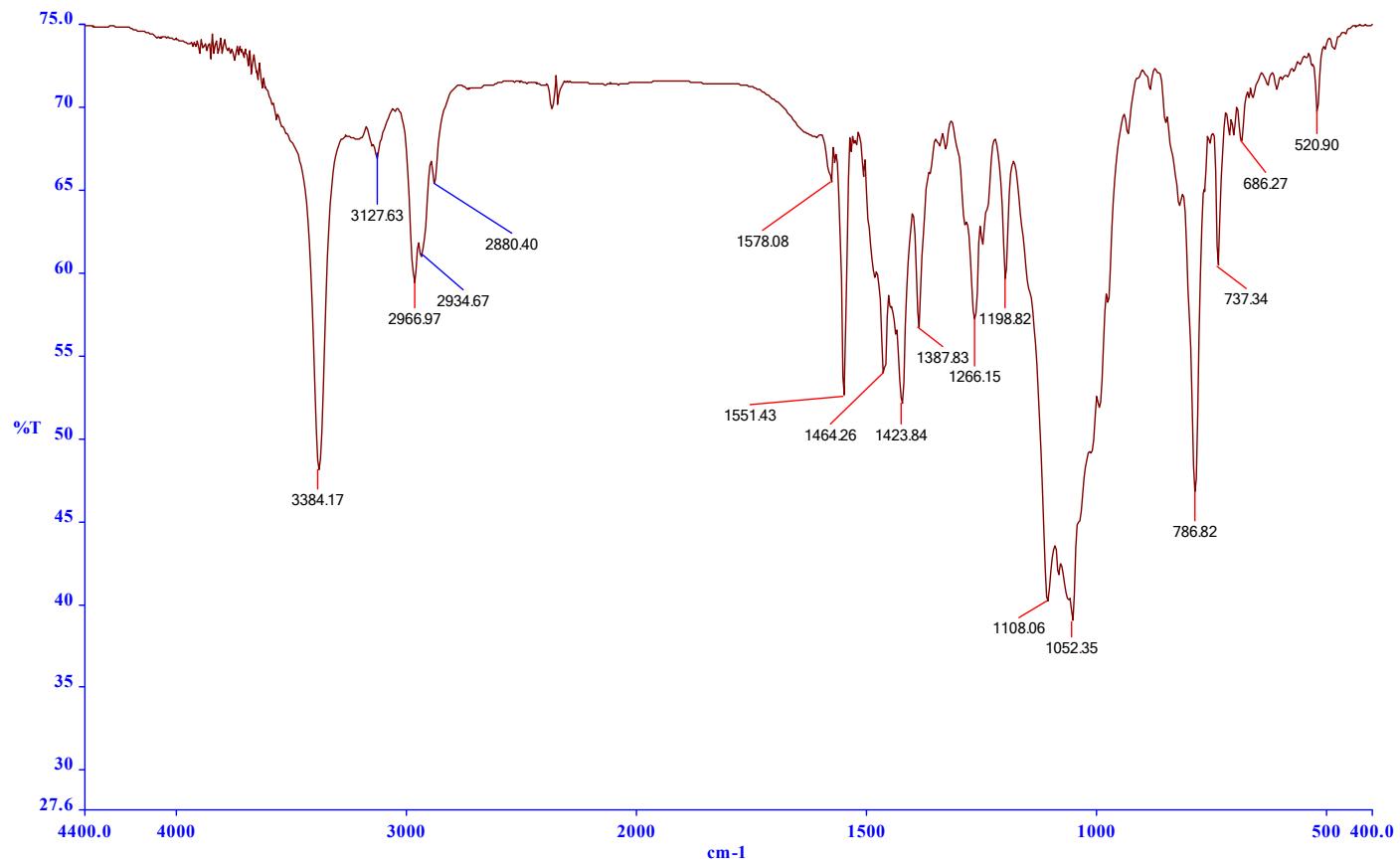


Figure S10: IR spectrum of silver(I) complex 4 recorded as a KBr disc.

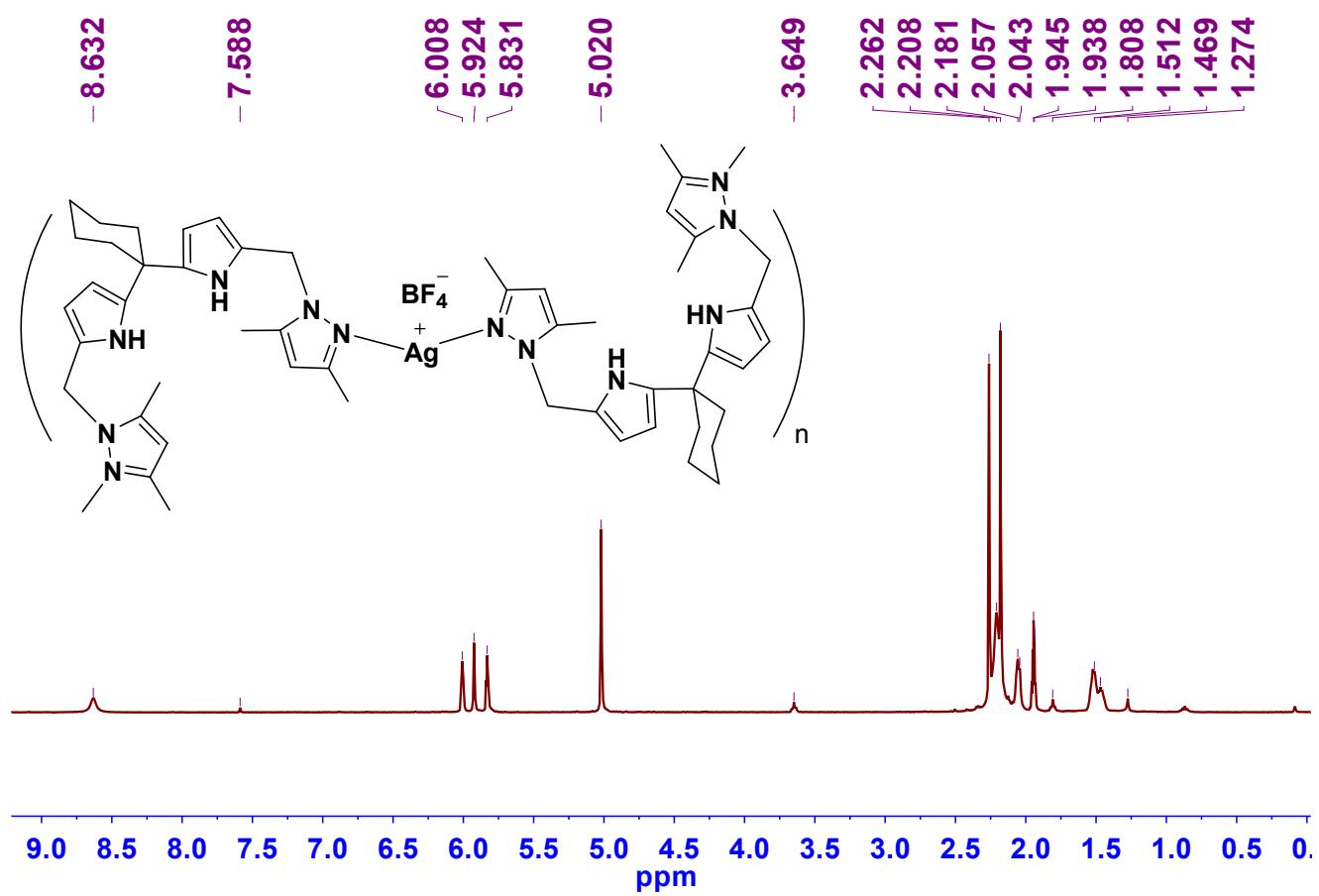


Figure S11: ^1H NMR (400 MHz) spectrum of silver(I) complex **5** in CD_3CN at room temperature.

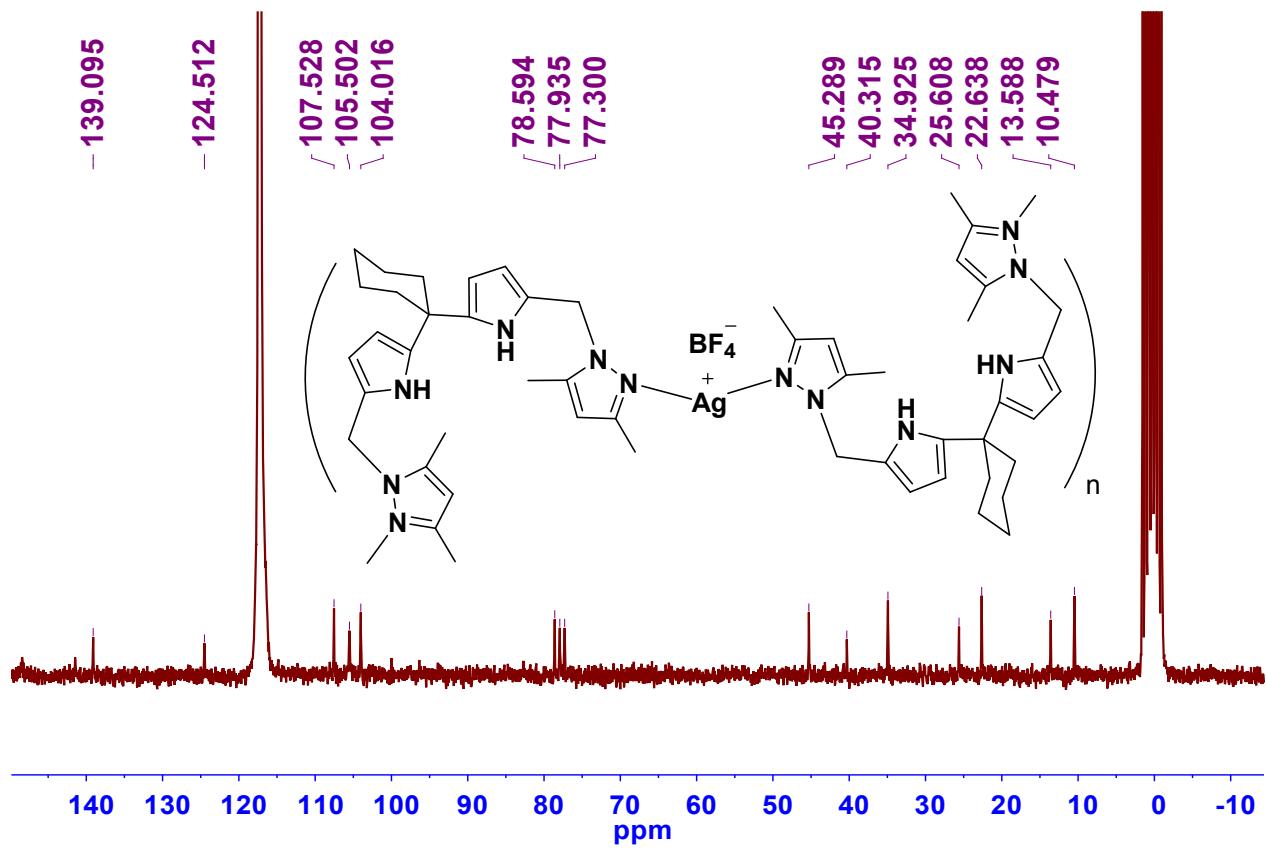


Figure S12: $^{13}\text{C}\{^1\text{H}\}$ NMR (50.3 MHz) spectrum of silver(I) complex **5** in CD_3CN at room temperature.

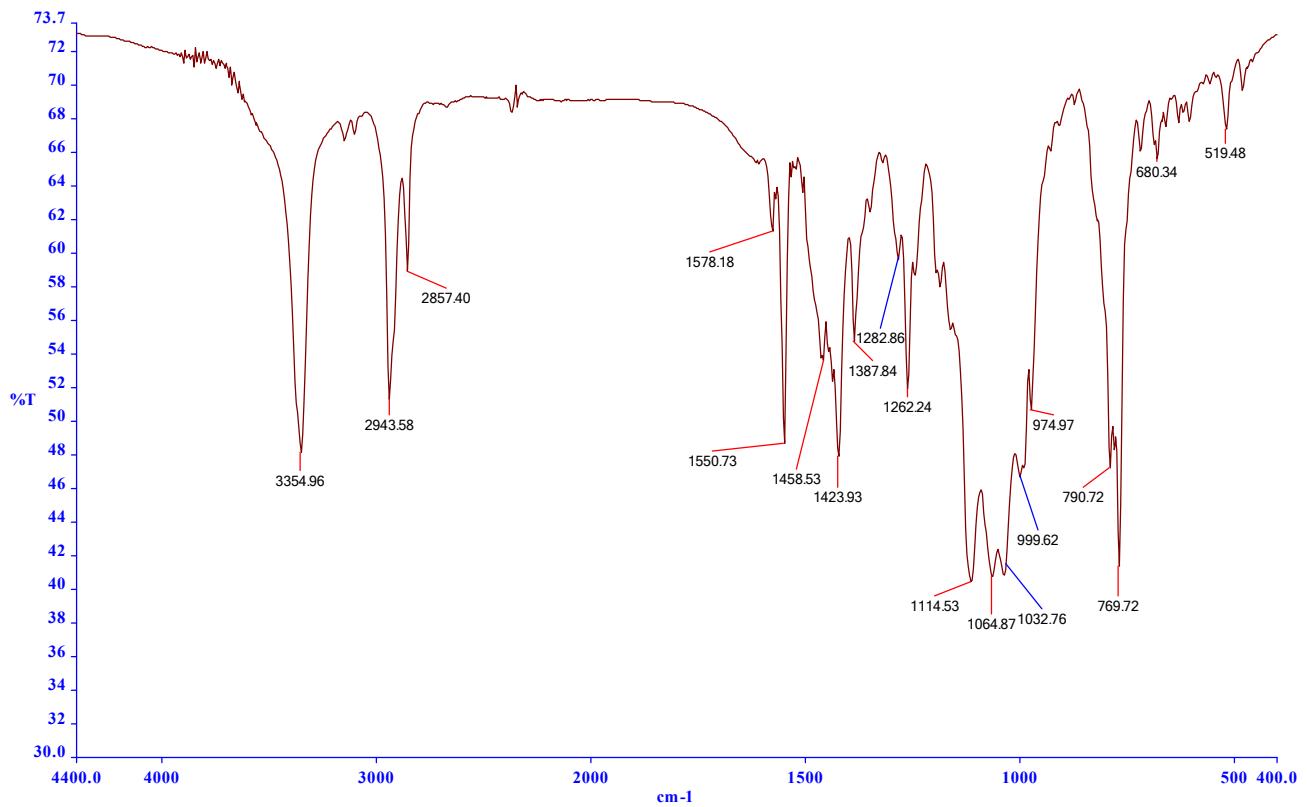


Figure S13: IR spectrum of silver(I) complex **5** recorded as a KBr disc

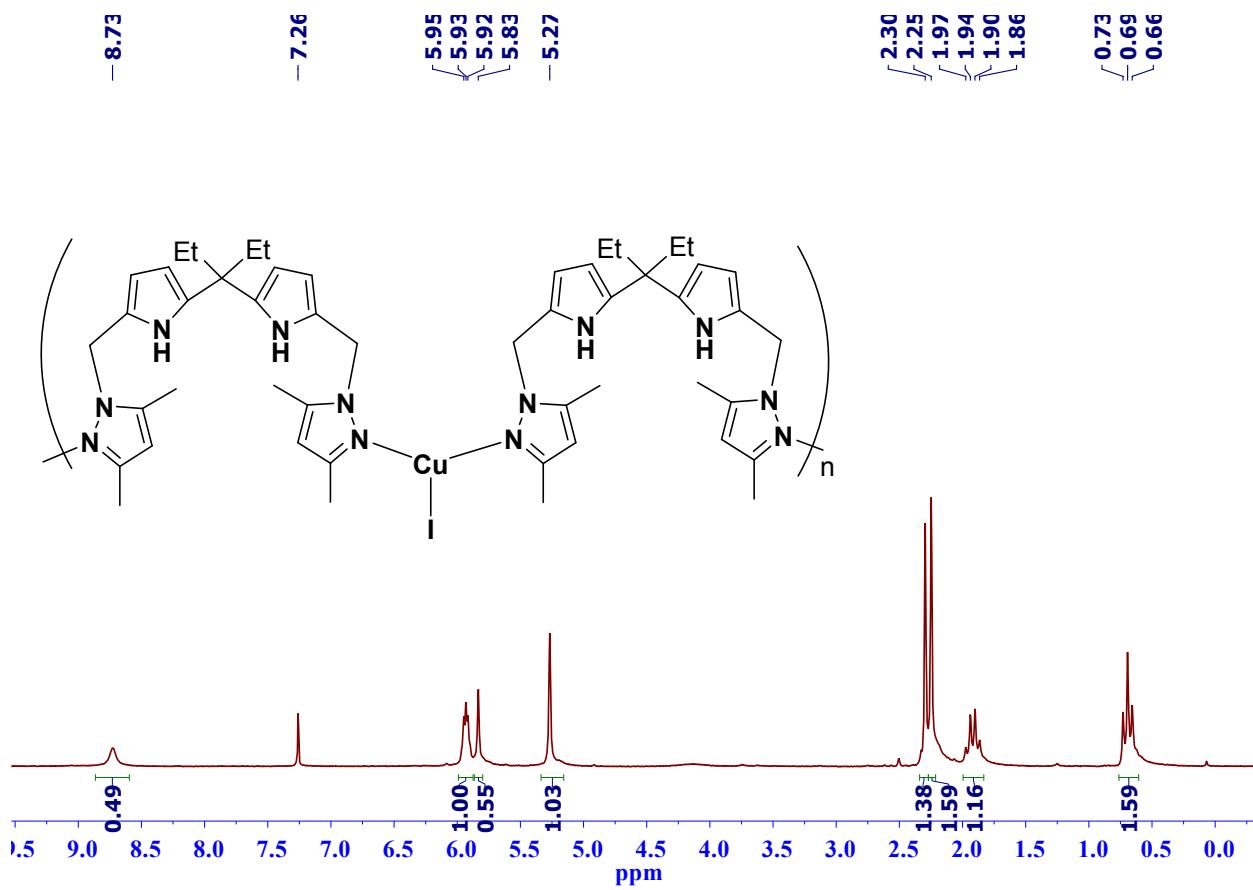


Figure S14: ^1H NMR (200 MHz) spectrum of copper(I) complex **6** in CDCl_3 at room temperature.

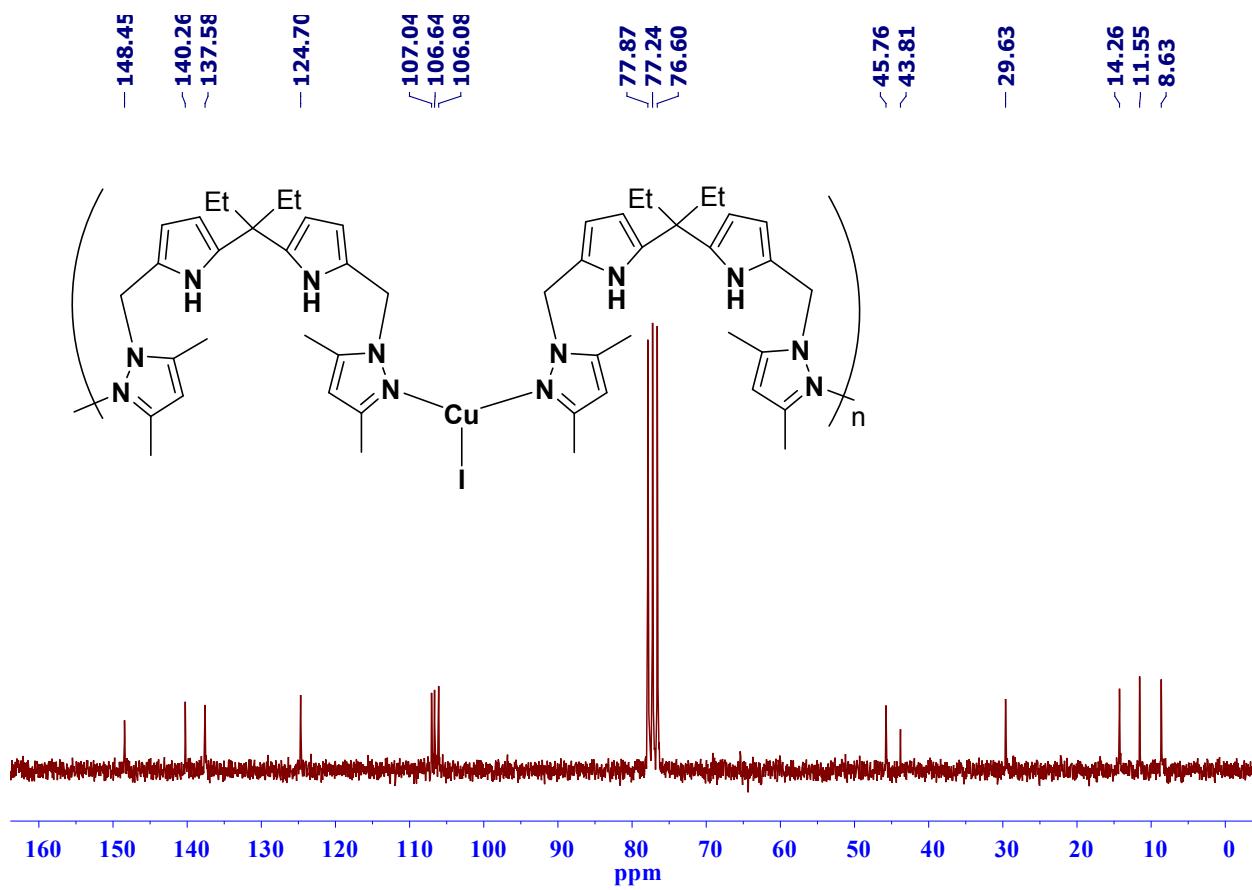


Figure S15: $^{13}\text{C}\{^1\text{H}\}$ NMR (50.3 MHz) spectrum of copper(I) complex **6** in CDCl_3 at room temperature.

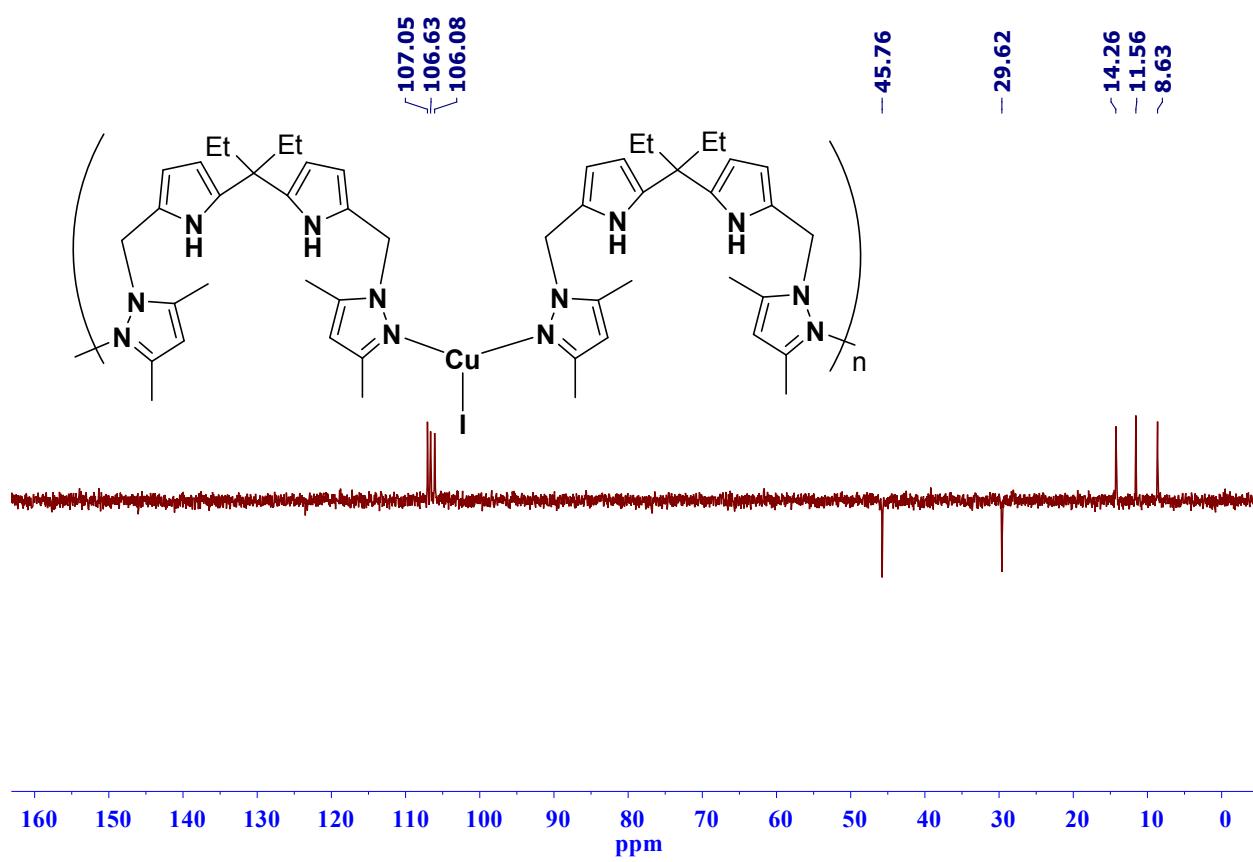


Figure S16: DEPT-135{¹H} NMR (50.3 MHz) spectrum of copper(I) complex **6** in CDCl₃ at room temperature.

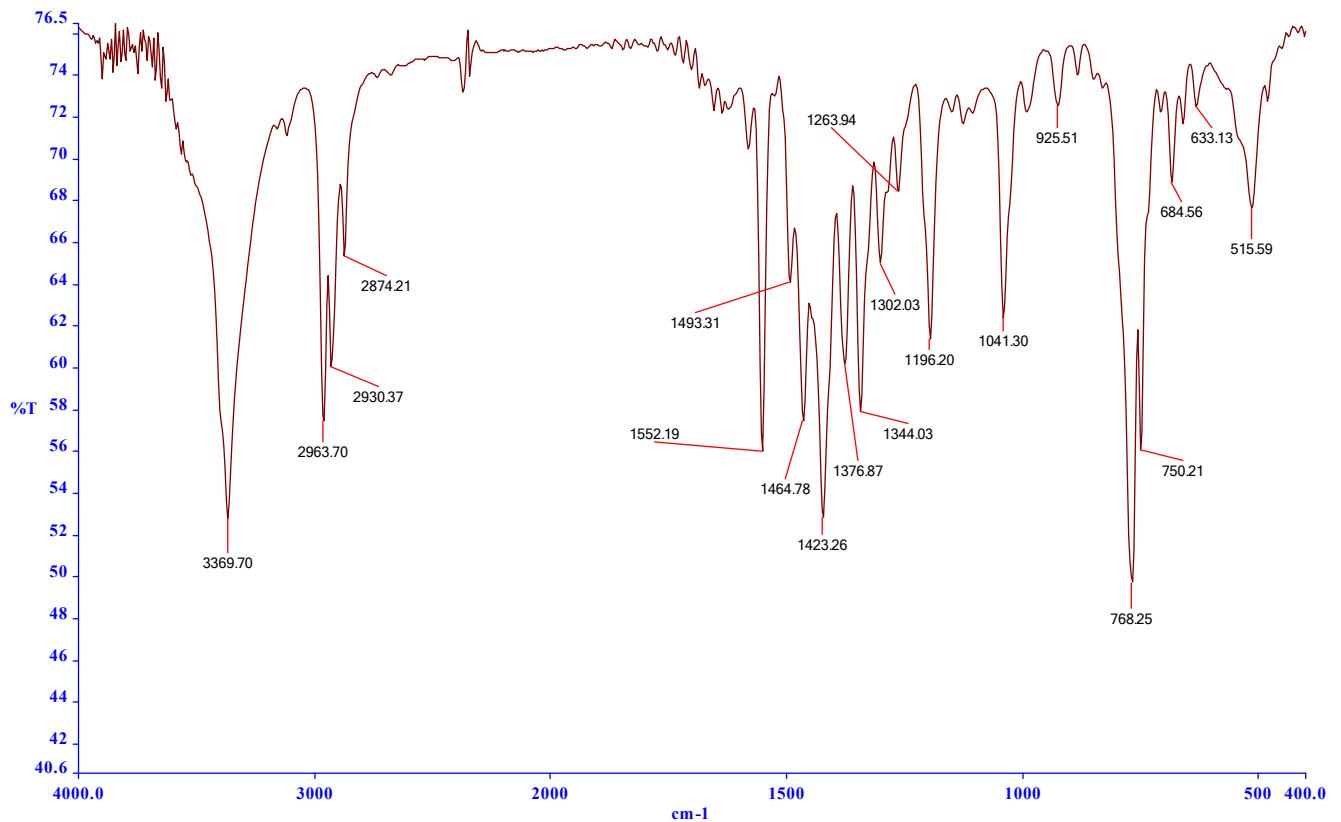


Figure S17: IR spectrum of copper(I) complex **6** recorded as a KBr disc.

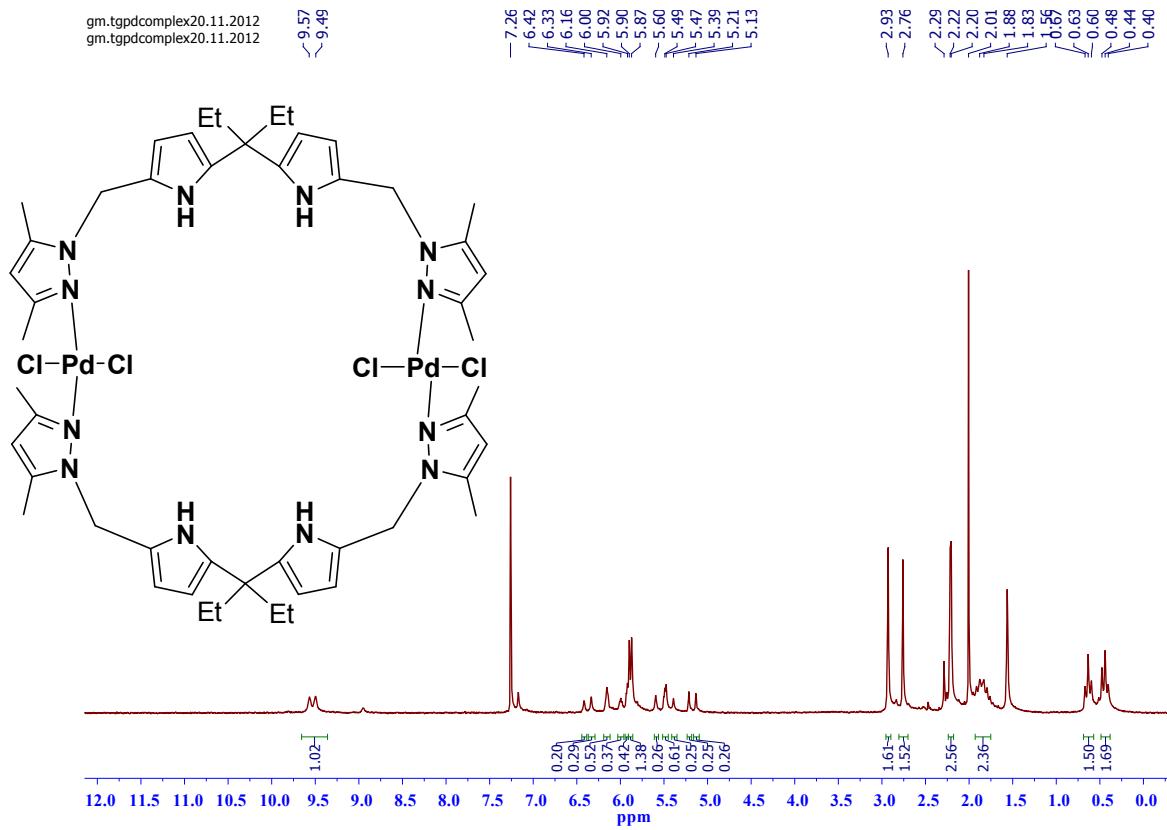


Figure S18: ^1H NMR (200 MHz) spectrum of palladium(II) complex 7 in CDCl_3 at room temperature.

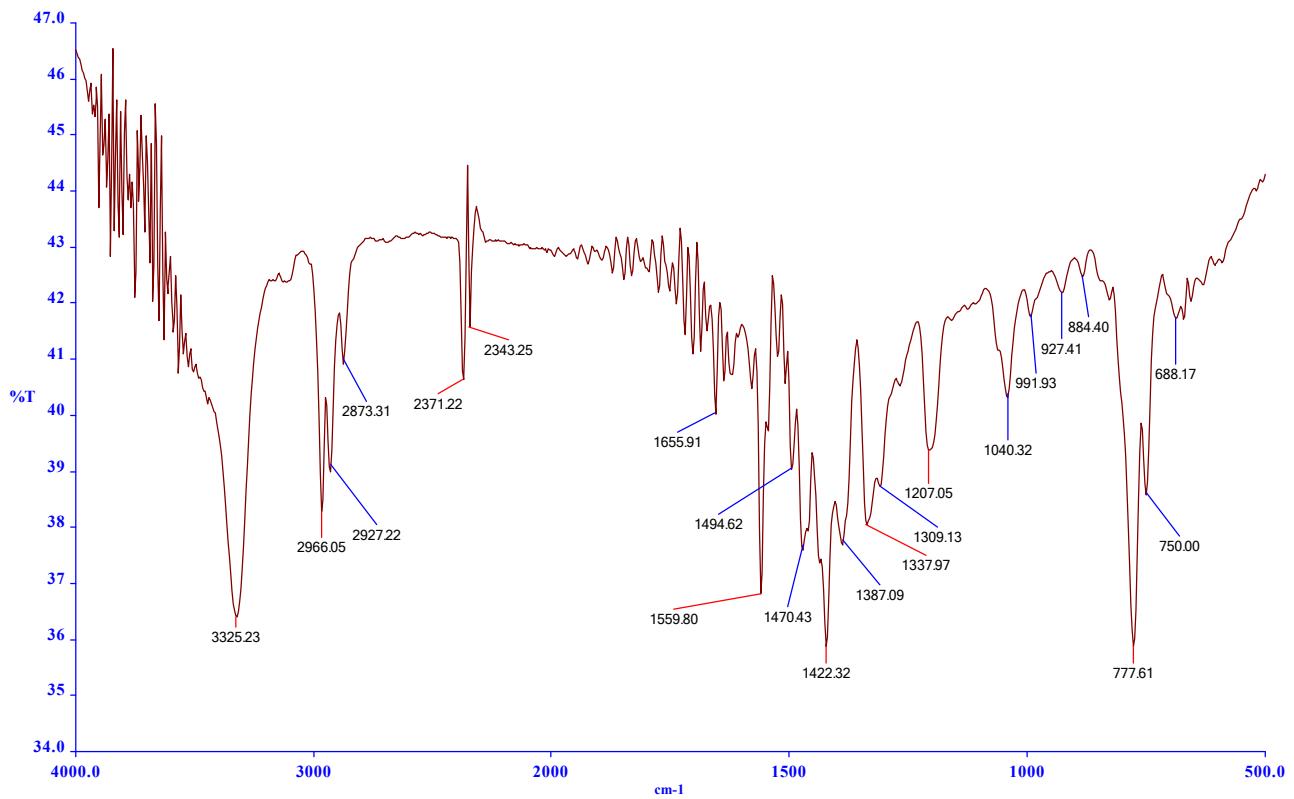


Figure S19: IR spectrum of palladium(II) complex **7** recorded as a KBr disc.

Synthesis of copper complex from the reaction of **L₂** with CuI:

To a suspension of CuI (0.08 g, 0.42 mmol) in THF (50 mL) was added **L₂** (0.18 g, 0.42 mmol). The resulting suspension was stirred at room temperature for 1 day, giving almost clear colorless solution. The solution was filtered and the solvent was removed. The resulting residue was washed with petroleum ether (10 mL × 2) to give a colorless solid (0.11 g).

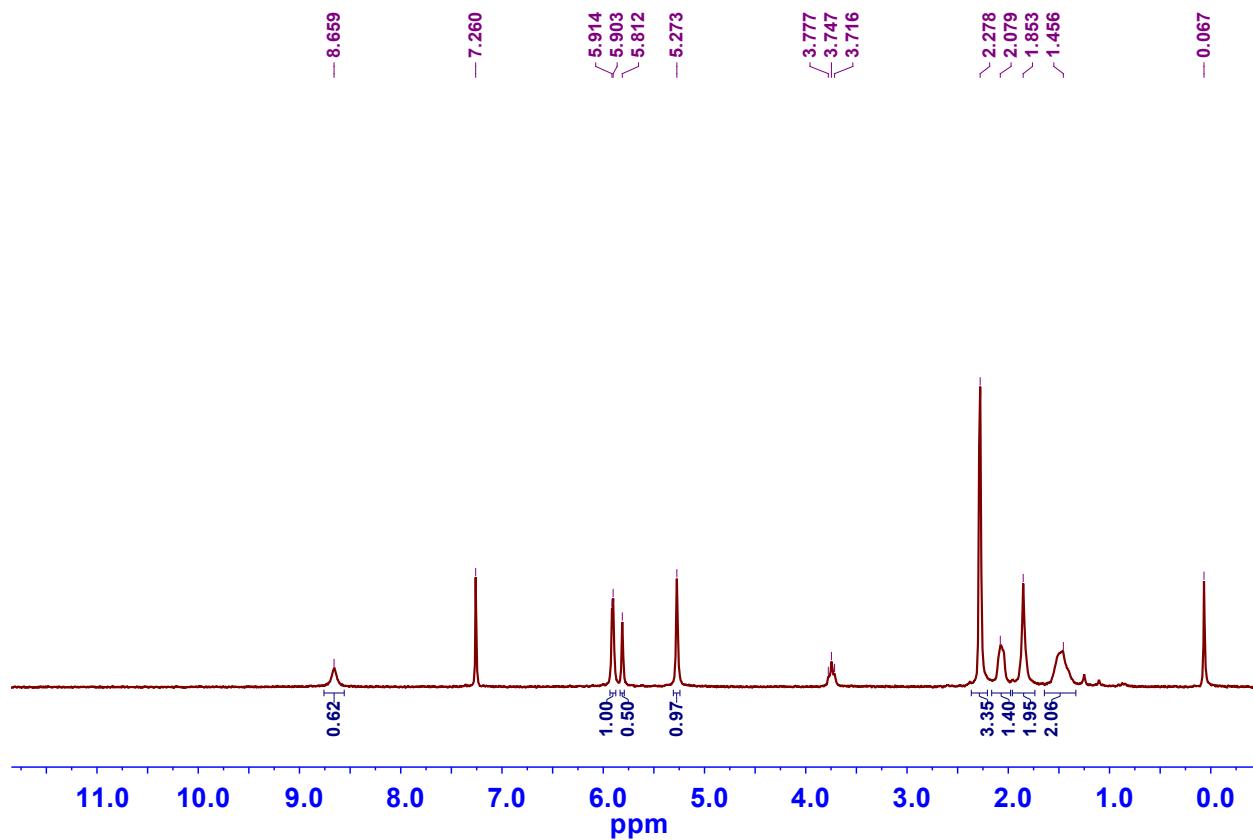


Figure S20: ¹H NMR (200 MHz) spectrum of the copper complex in CDCl₃ obtained from the reaction of **L₂** with CuI at room temperature. This spectrum shows THF resonances as well, which is from the reaction medium.

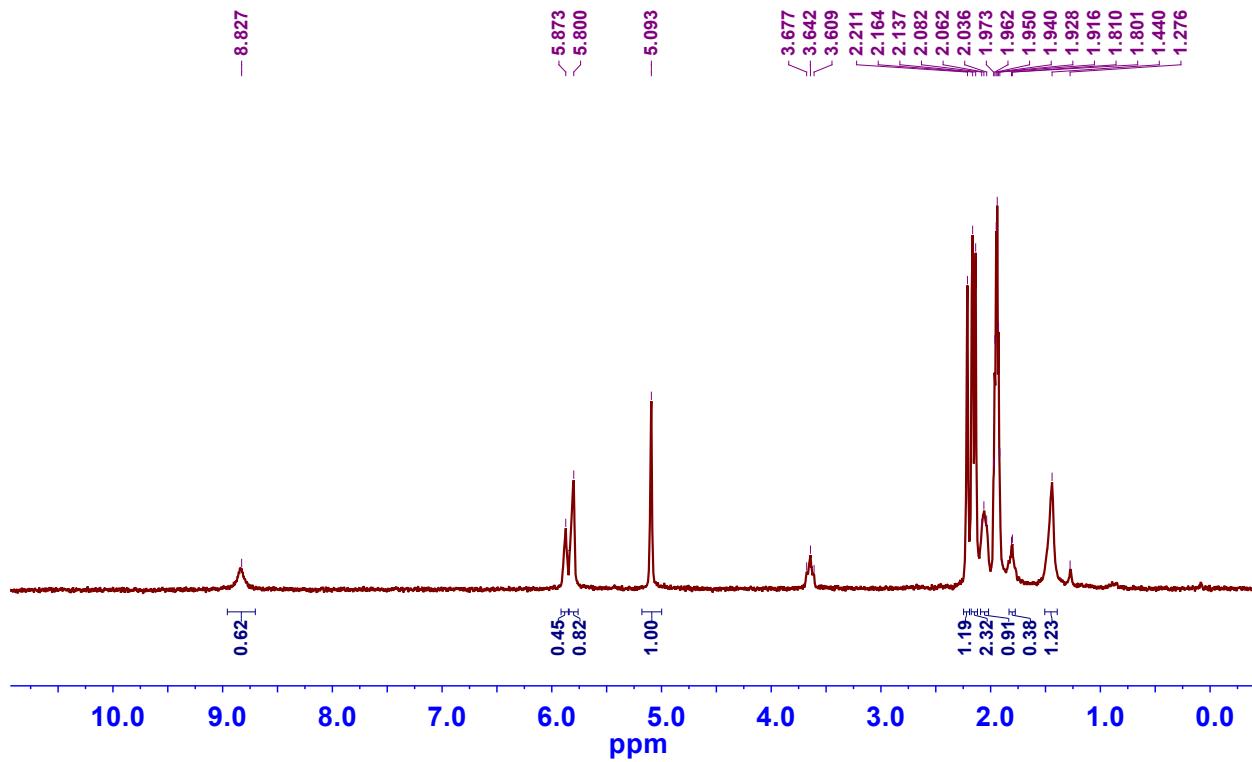


Figure S21: ^1H NMR (200 MHz) spectrum of the copper complex in CD_3CN obtained from the reaction of L_2 with CuI at room temperature. This spectrum shows THF resonances as well, which is from the reaction medium.

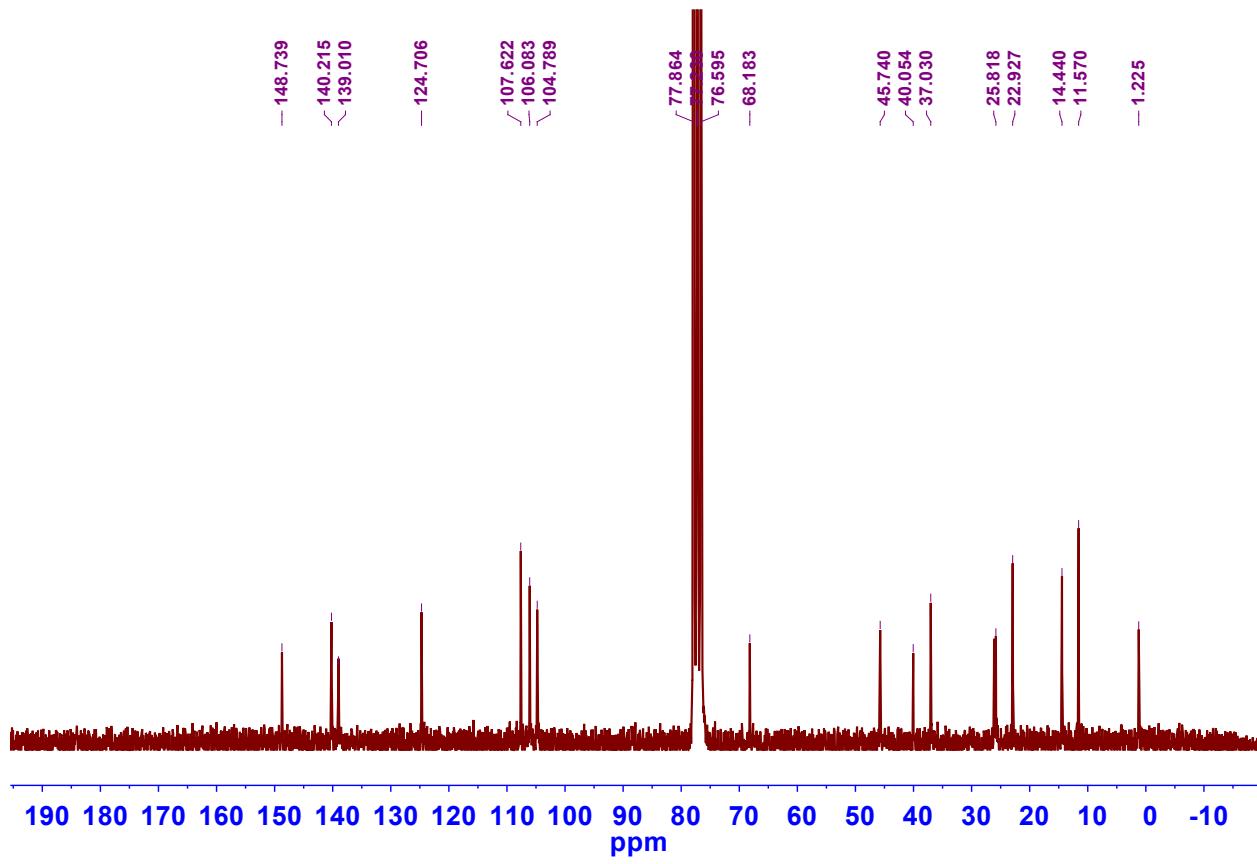


Figure S22: $^{13}\text{C}\{^1\text{H}\}$ NMR (50.3 MHz) spectrum of copper(I) complex in CDCl_3 obtained from the reaction of **L₂** with CuI at room temperature. The resonances at 68.18 and 28.82 ppm are due to THF which is from the reaction medium. The resonance at 1.22 ppm is due to impurity.

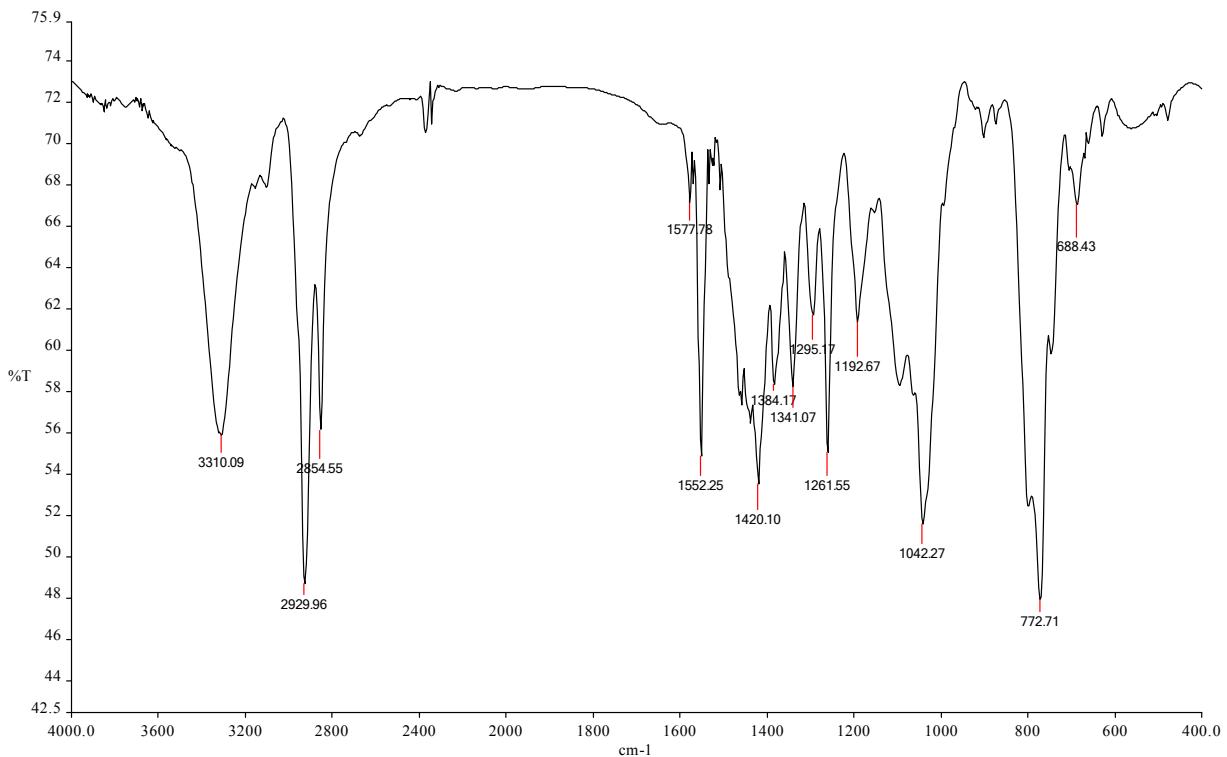


Figure S23: IR spectrum of the copper complex obtained from the reaction of **L₂** with CuI recorded as a KBr disc.