Electronic Supporting information

Novel heteroleptic copper(I) complexes merging the chelating 1,2-bis-diphenyldiphosphine and various L^X type coligands

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X-Ray crystal structure determination. Single crystals were selected, mounted and transferred into a cold nitrogen gas stream. Intensity data was collected with a Bruker Kappa-APEX2 system using micro-source Cu-Kα radiation. Unit-cell parameters determination, data collection strategy, integration and absorption correction were carried out with the Bruker APEX2 suite of programs. The structures were solved with SIR92[C1] (**2**) or SIR97[C1] (**2**) and refined anisotropically by full-matrix least-squares methods with SHELXL[C2] using WinGX.[C3] Absolute structure for **(2)** was determined by anomalous scattering effects analysis.[C4] Both structures were deposited at the Cambridge Crystallographic Data Centre with numbers CCDC 1942668 and 1943248. These can be obtained free of charge via www.ccdc.cam.ac.uk.

Crystal data for 2. $C_{40}H_{32}CuNOP_2$, orthorhombic P m n 2_1, a = 17.3563(2) Å, b = 11.8638(2) Å, c = 8.1509(1) Å, α = β = γ = 90°, V = 1678.37(4) Å^3, Z = 2, yellow needle 0.9 x 0.15 x 0.02 mm, μ = 2.064 mm^{-1}, min / max transmission = 0.43 / 1.00, T= 200(1) K, λ = 1.54178 Å, θ range = 3.73° to 66.56°, 10246 reflections measured, 2286 independent, R_{int} = 0.0295, completeness = 0.991, 224 parameters, 1 restraint, Flack x = -0.00(2), final R indices R1 [I>2σ(I)] = 0.0232 and wR2 (all data) = 0.0632, GOF on F^2 = 1.046, largest difference peak / hole = 0.20 / -0.20 e.Å^{-3}.

Crystal data for 3. $C_{37}H_{30}CuNO_2P_2$, monoclinic P 2_1/n, a = 8.3072(2) Å, b = 18.5057(4) Å, c = 19.9706(4) Å, α = γ = 90°, β = 94.867(1)° ,V = 3059.02(12) Å^3, Z = 4, colourless needle 0.15 x 0.03 x 0.02 mm, μ = 2.270 mm^{-1}, min / max transmission = 0.68 / 0.75, T= 200(1) K, λ = 1.54178 Å, θ range = 3.27° to 68.52°, 26598 reflections measured, 5504 independent, R_{int} = 0.0318, completeness = 0.980, 389 parameters, 0 restraints, final R indices R1 [I>2σ(I)] = 0.0299 and wR2 (all data) = 0.0767, GOF on F^2 = 1.020, largest difference peak / hole = 0.29 / -0.30 e.Å^{-3}.

C1- A. Altomare, G. Cascarano, C. Giacovazzo, A. Guagliardi , *J. Appl. Cryst.* **1993**, 26, 343-350.
C2- G. M. Sheldrick, *Acta Cryst. C* **2015**, 71, 3-8.
C3- L.J. Farrugia, *J. Appl. Cryst.* **2012**, 45, 849–854.
C4- H. D. Flack and G. Bernardinelli, *J. Appl. Cryst.* **2000**, 33, 1143-1148.

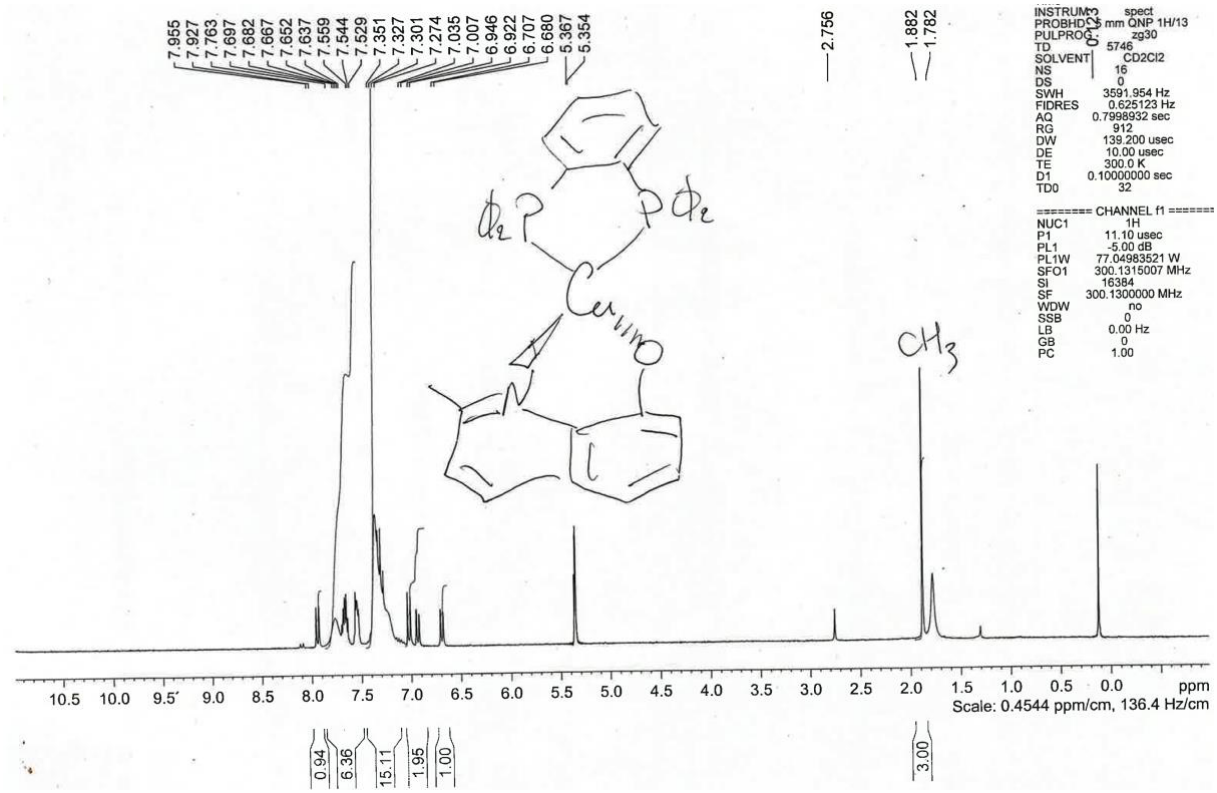

Figure S1: ^{1}H-NMR spectrum of compound [Cu(Me-Q)(dppb)] (**2**) in CD_2Cl_2

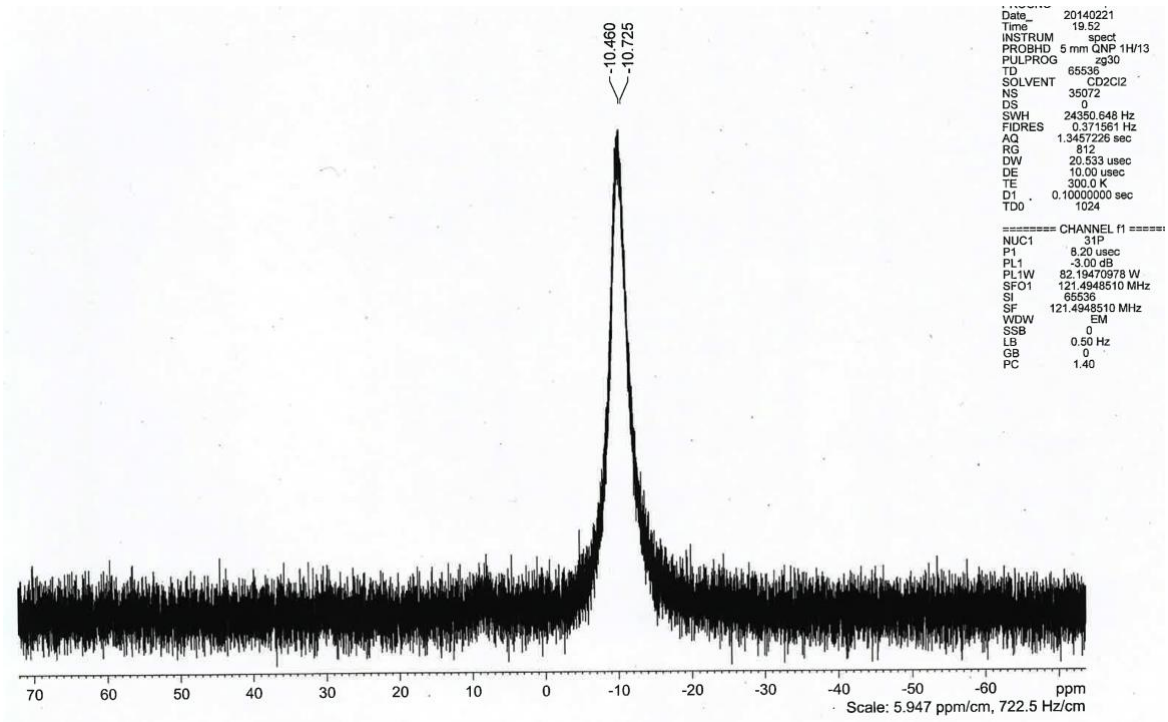

Figure S2: ^{31}P-NMR spectrum of compound [Cu(Me-Q)(dppb)] (**2**) in CD_2Cl_2

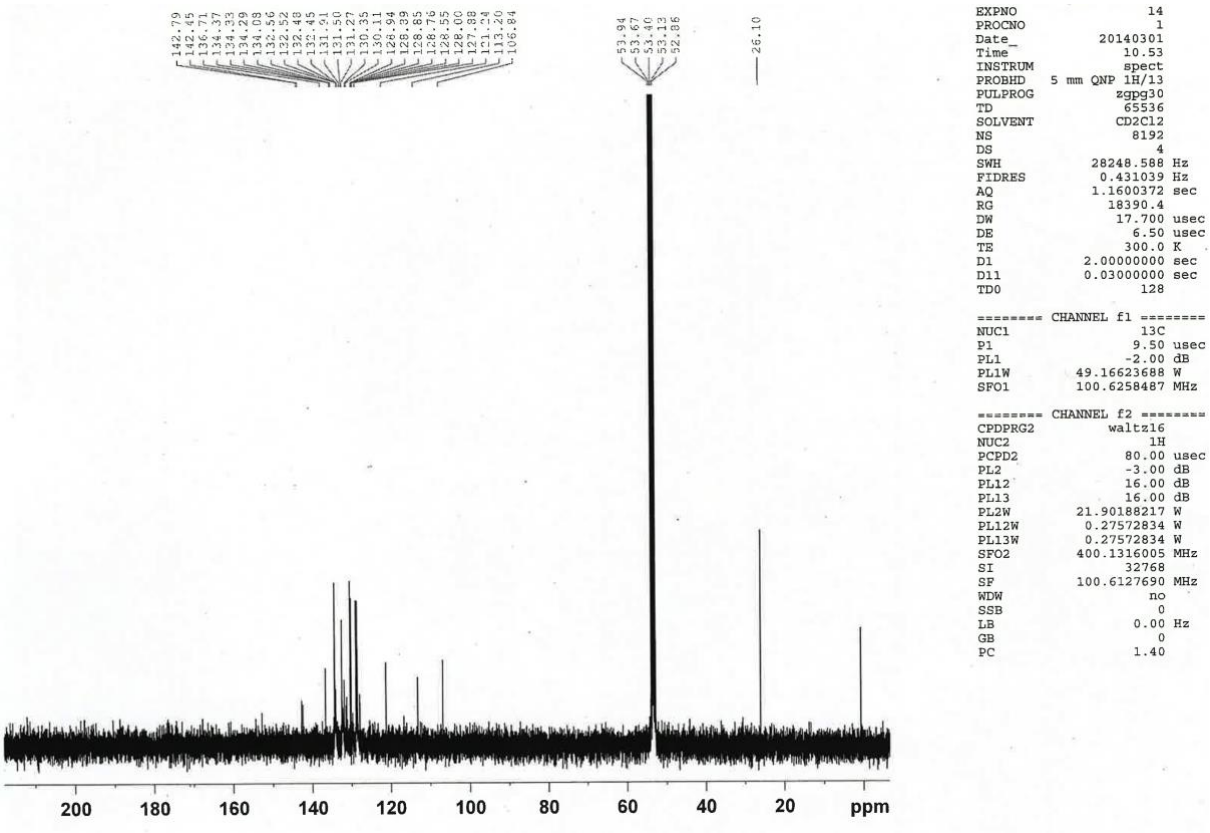

Figure S3: ^{13}C-NMR spectrum of compound [Cu(Me-Q)(dppb)] (**2**) in CD_2Cl_2

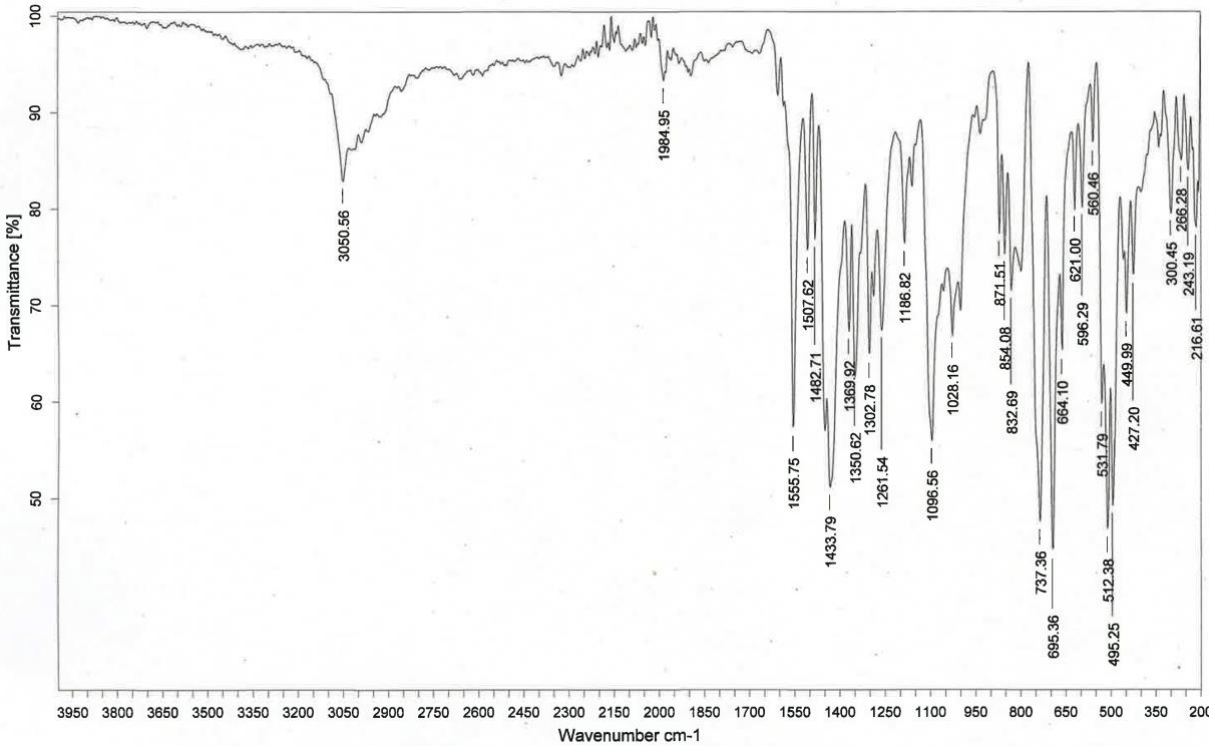

Figure S4: ATR-Infrared spectrum of compound [Cu(Me-Q)(dppb)] (**2**)

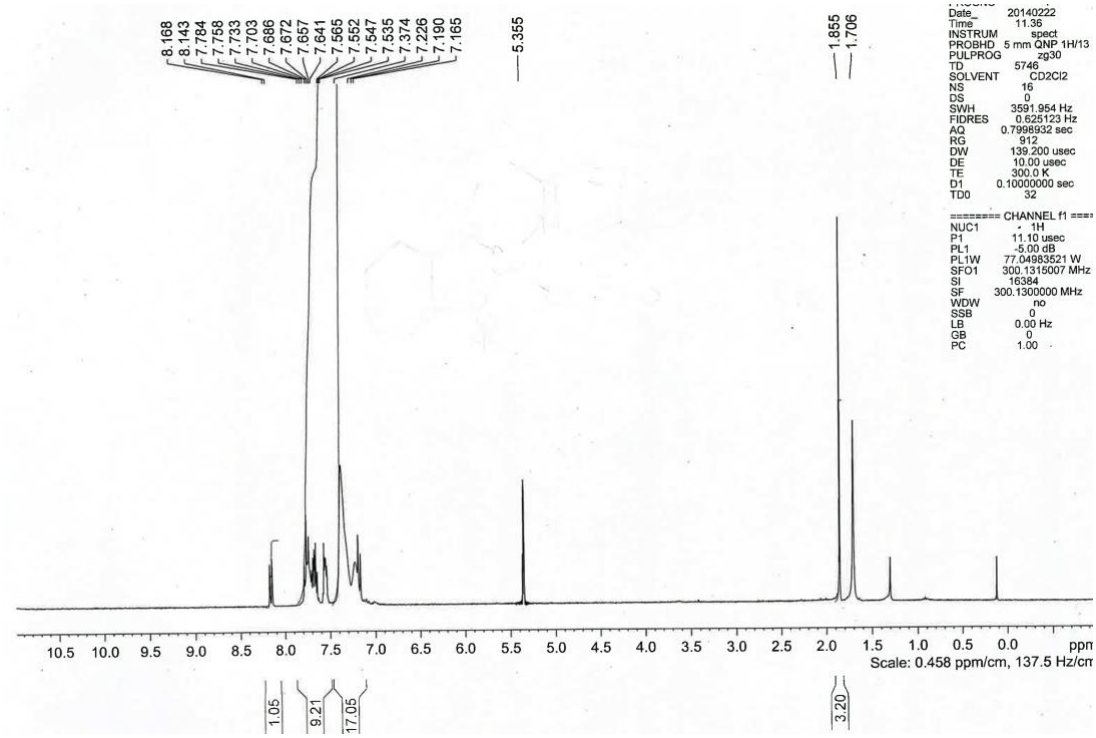

Figure S5: ^{1}H-NMR spectrum of compound [Cu(Me-Pic)(dppb)] (**3**) in CD_2Cl_2

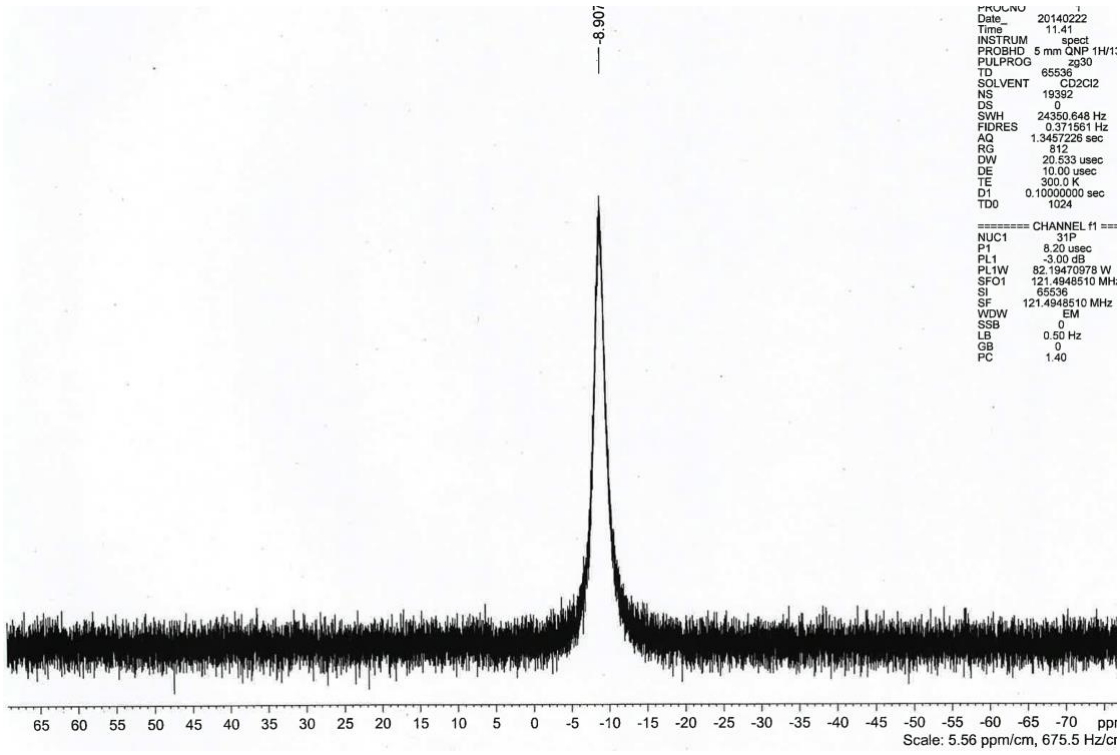

Figure S6: ^{31}P-NMR spectrum of compound [Cu(Me-Pic)(dppb)] (**3**) in CD_2Cl_2

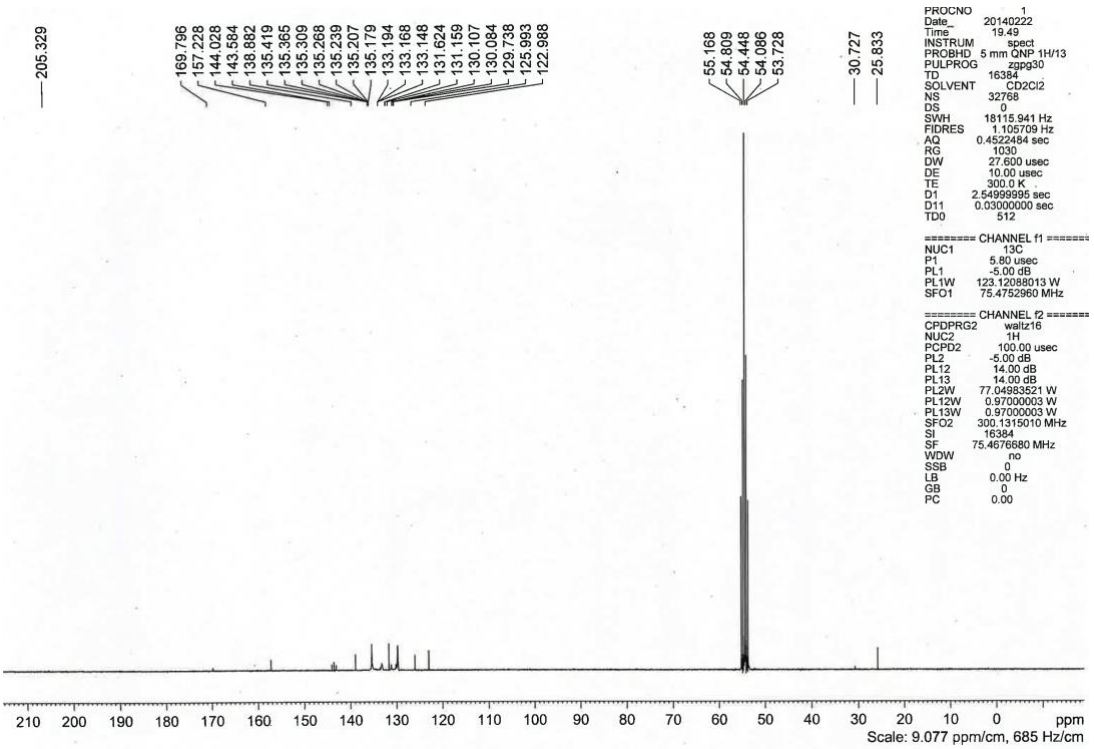

Figure S7: ^{13}C-NMR spectrum of compound [Cu(Me-Pic)(dppb)] (**3**) in CD_2Cl_2

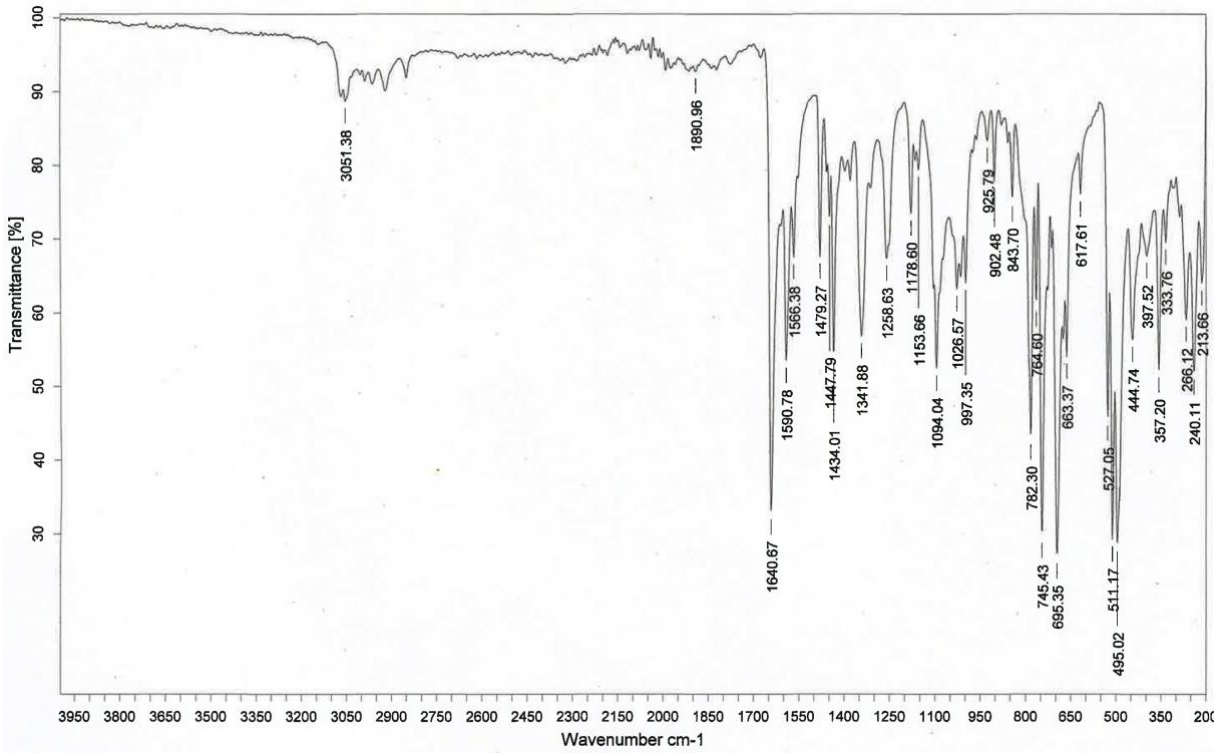

Figure S8: ATR-Infrared spectrum of compound [Cu(Me-Pic)(dppb)] (**3**)

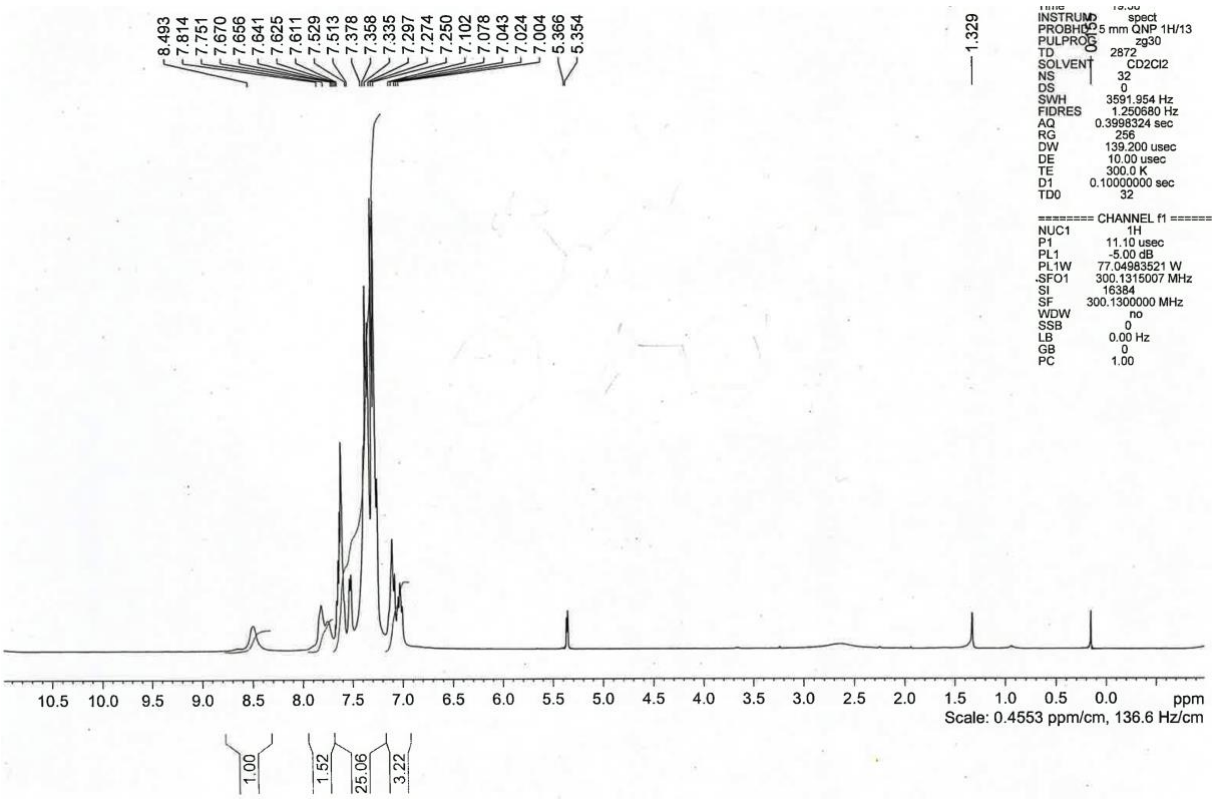

Figure S9: ^{1}H-NMR spectrum of compound [Cu(pbim)(dppb)] (**4**) in CD_2Cl_2

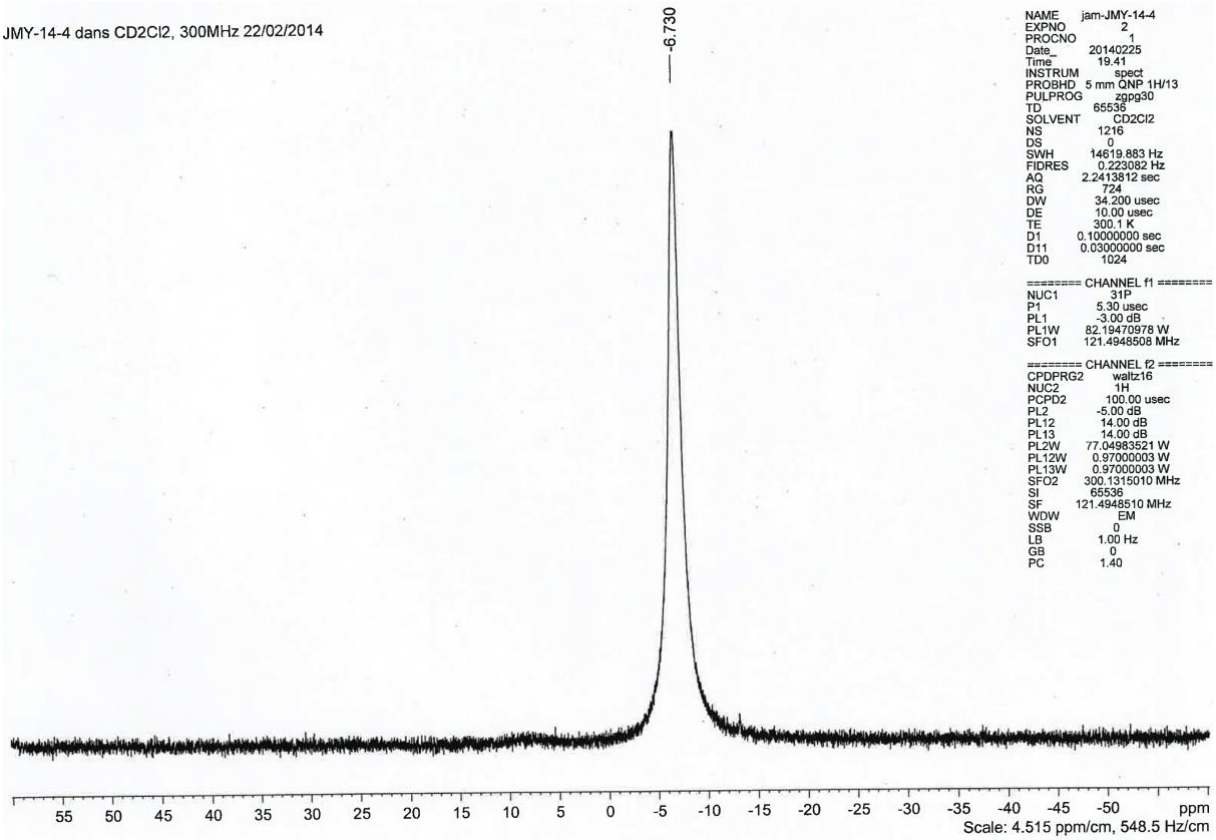

Figure S10: ^{31}P-NMR spectrum of compound [Cu(pbim)(dppb)] (**4**) in CD_2Cl_2

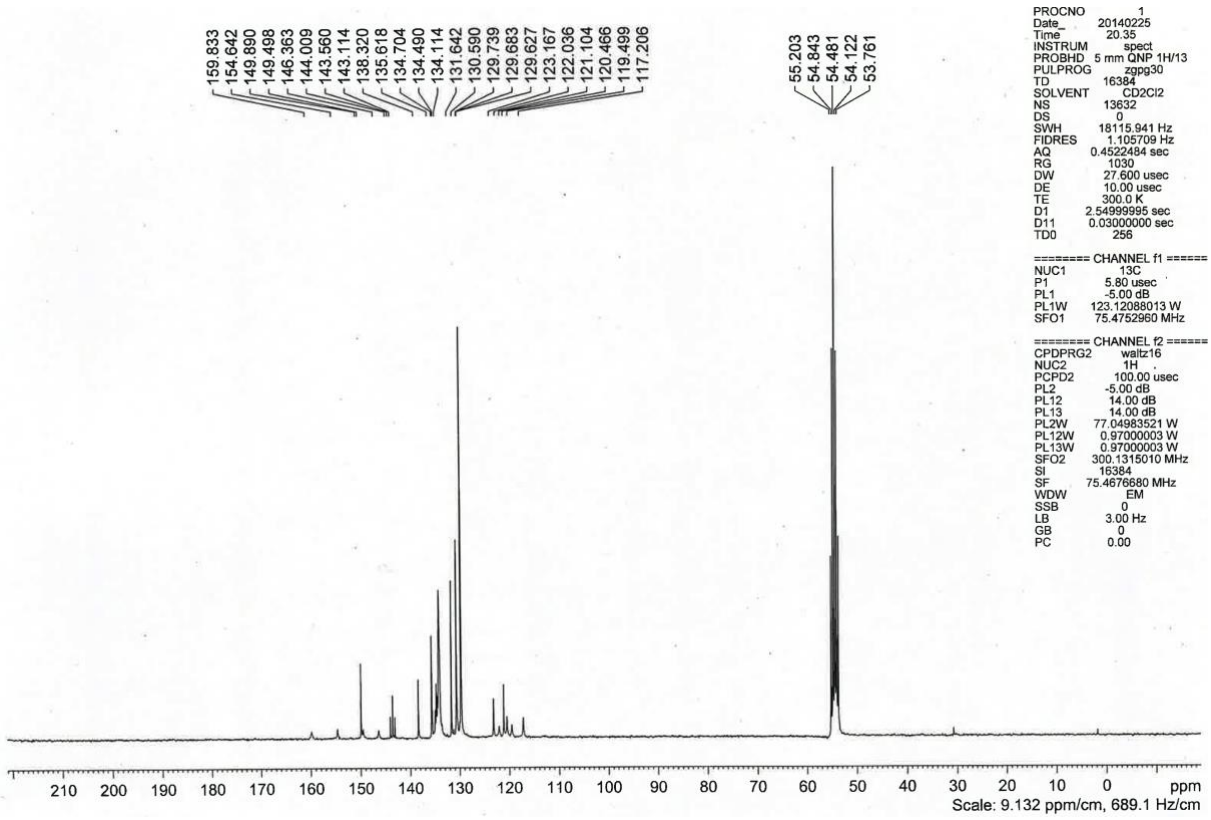

Figure S11: ^{13}C-NMR spectrum of compound [Cu(pbim)(dppb)] (**4**) in CD_2Cl_2

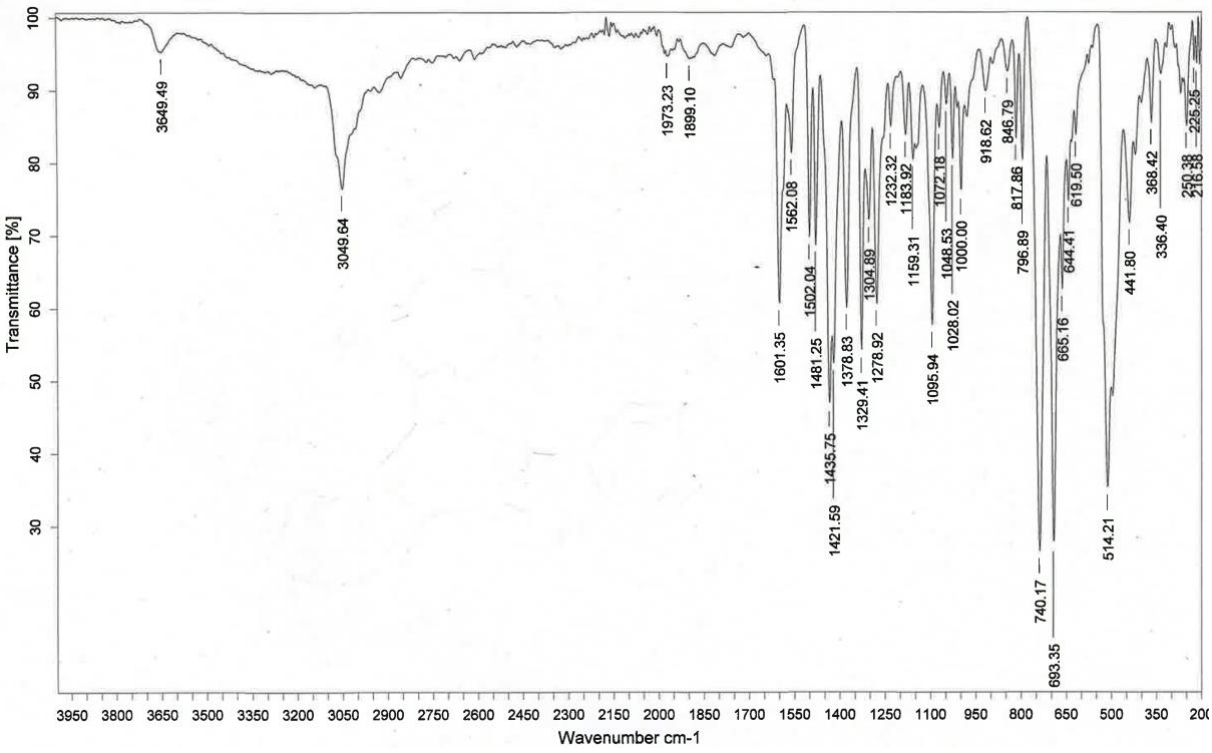

Figure S12: ATR-Infrared spectrum of compound [Cu(pbim)(dppb)] (**4**)