New Bisoxazoline Copper(II) and Platinum(II) Complexes

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Abstract

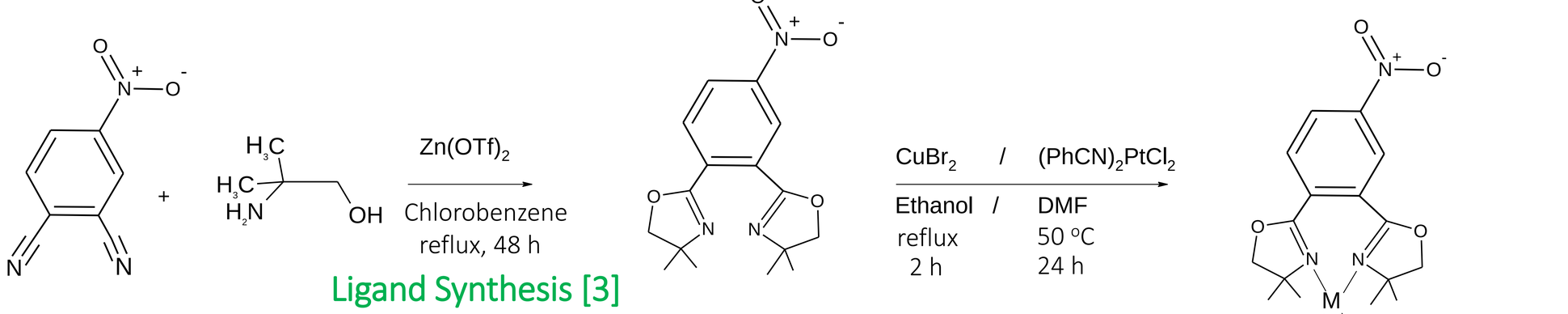
This communication reports on the synthesis and characterization of new copper(II) and Platinum(II) bisoxazoline complexes. The Ligand (2,2'-(4-nitro-1,2-phenylene)bis(4,4-dimethyl-4,5-dihydro-1,3-oxazole)) (NO_2BOX) was synthesized following a procedure reported earlier by our group [1] and characterized by NMR and IR spectroscopy. The complexes (NO_2BOX)$CuBr_2$ (A) and (NO_2BOX)$PtCl_2$ (B) were synthesized by reacting the ligand with stoichiometric amounts of $CuBr_2$ and $(PhCN)_2PtCl_2$, respectively. In addition to the characterization by IR and UV-Vis. spectroscopy, and elemental analysis, A and B were characterized respectively by ^1H and ^{13}C NMR, and Electron Paramagnetic Resonance. The single crystal X-ray structure of complex B was determined.

Keywords: Bisoxazoline; copper(II); platinum(II); X-ray crystal structure

I. Introduction

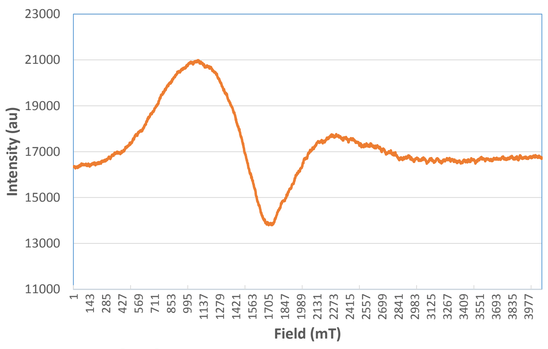
Bis(oxazolines) (BOX) ligands have attracted considerable attention in coordination chemistry mostly for applications in asymmetric catalysis [2]. The isolated metal complexes based on the BOX ligand (2,2'-(1,2-phenylene)bis(4,4-dimethyl-4,5-dihydro-1,3-oxazole)) and its substitution derivatives are scarce in literature [3]. In this project, we aimed at investigating part of the coordination chemistry of the nitro-substituted ligand with Platinum(II) and copper(II) metal ions. We present herein our results on the synthesis and characterization of two new complexes (NO_2BOX)$CuBr_2$ (A) and (NO_2BOX)$PtCl_2$ (B).

II. Synthesis

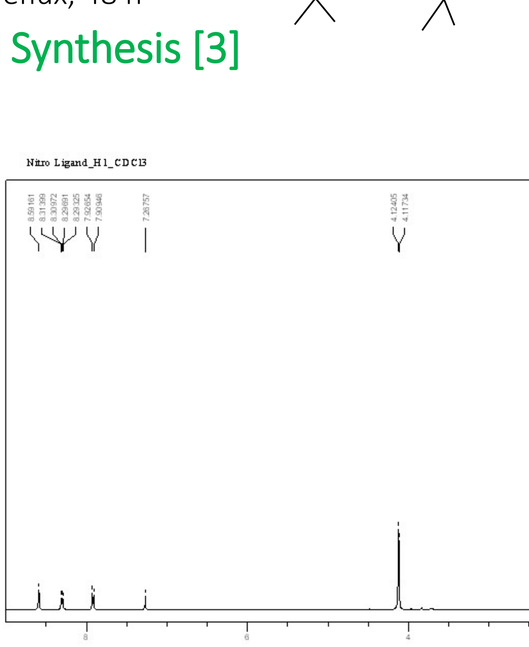


Ligand Synthesis [3]

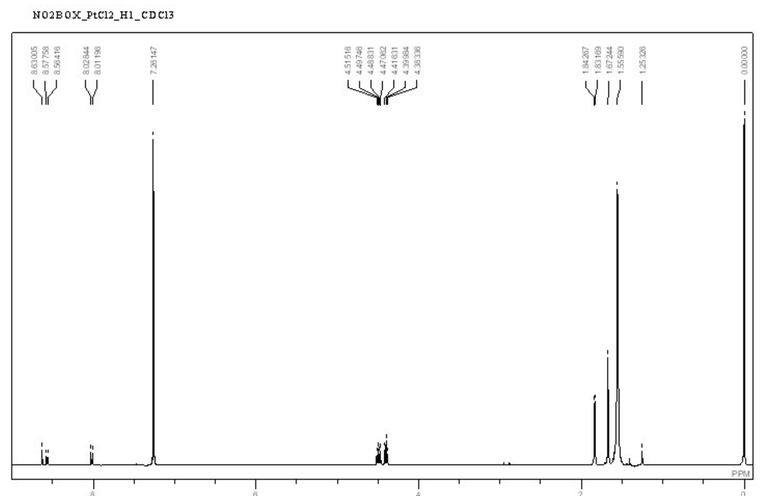
III. Characterization



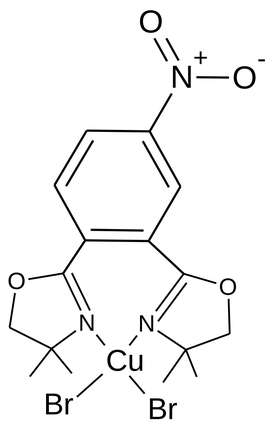
Solid state EPR spectrum of complex A
(g = 2.1625)



^1H NMR of ligand NO_2BOX



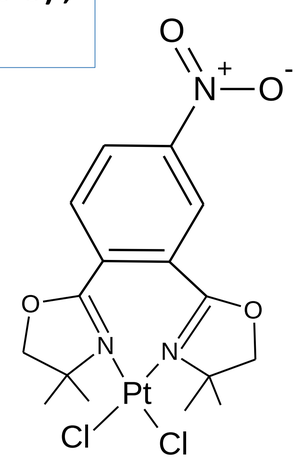
^1H NMR of complex B



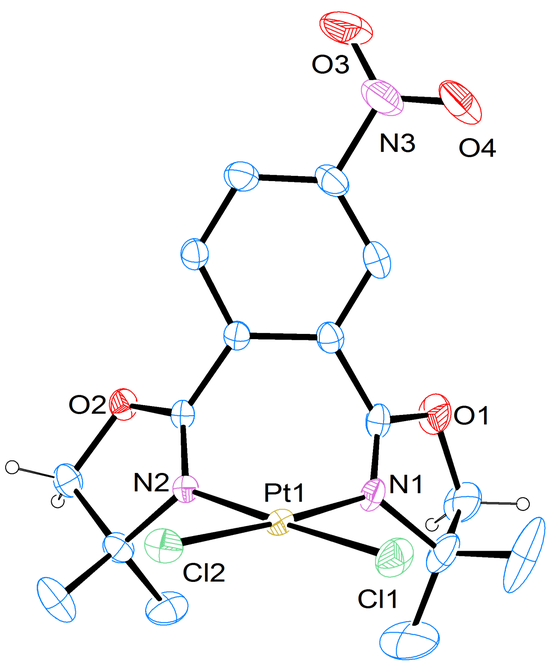
Complex A

ν(cm^{-1}): 1650s (C=N) ; 1528s, 1350s (NO) ; 1105m ; 1086s (C-O) ; 989m ; 965s ; 847m ; 716s

Characteristic IR frequencies of ligand NO_2BOX



Complex B



X-ray structure of complex B

Mid-IR ν(cm^{-1}): 1632s, 1659s (C=N) ; 1540s, 1351s (NO) ; 1130m (C-O) ; 1065m ; 954s ; 714m

Far-IR ν(cm^{-1}): 325 (Cu-N) ; 182 , 151 (Cu-Br)

Characteristic IR frequencies of complex A

Mid-IR ν(cm^{-1}): 1634s (C=N); 1534s ; 1350m (NO) ; 1131m (C-O) ; 1061m ; 948m ; 710m

Far-IR ν(cm^{-1}): 563, 497 (Pt-N) ; 413, 323 (Pt-Cl) ; 253 (δ N-Pt-N)

Characteristic IR frequencies of complex B

IV. Conclusion and future work

Two new complexes (NO_2BOX)$CuBr_2$ (A) and (NO_2BOX)$PtCl_2$ (B) were synthesized and characterized. Complex A is a potential catalyst in a variety of important reactions including C-C and C-Heteroatom coupling reactions. Complex B is a potential anticancer agent.
Future work may include catalytic activity studies of A and cytotoxic activity investigation of B.

References

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[2] Gómez, M.; Muller, G.; Rocamora, M. *Coord. Chem. Rev.* 1999, 769, 193
[3] Rosa Silva, A.; Lourenço M. A. O.; Mayoral,A.; Diaz, I and Ferreira P. *Eur. J. Inorg. Chem*. 2016,413