(NHC) Cu(I) Complexes bearing Dipyridylamine ligands : Synthesis, Structural, Photoluminescent Studies and Applications in Luminescent Materials.

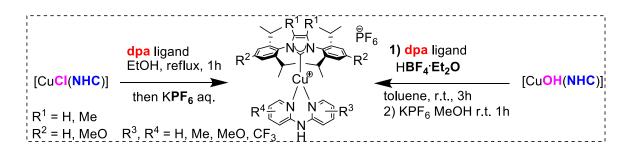
<u>Margaux ELIE</u>,^[a] Fabien SGUERRA,^[b] Florent DI MEO,^[c] Michael D. WEBER,^[d] Ronan MARION,^[a] Jean-Luc RENAUD,^[a] Mathieu, LINARES,^{[c],*} Matthieu HAMEL,^{[b],*} Rubèn D. COSTA ,^{[d],*} and Sylvain GAILLARD^{[a],*}

[a] LCMT, Normandie University, CNRS, UMR 6507, ENSICAEN, Caen, France

[b] CEA, LIST, Saclay, Laboratoire Capteurs et Architectures Electroniques, F-91191, Gif-sur-Yvette Cedex, France

- [c] Department of Physics, Chemistry and Biology SE-581 83, Linköping University, Sweden
 [d] Department of Chemistry and Pharmacy at the University of Erlangen-Nuremberg, 9
- [d] Department of Chemistry and Pharmacy at the University of Erlangen-Nuremberg, 91058 Erlangen, Germany

We present in this communication the synthesis of new cationic tricoordinated copper complexes bearing bidentate dipyridylamine (dpa) ligands and NHC as ancillary ligands [Cu(NHC)(HDPA)][X].^(1,2) These copper complexes have been fully characterized by NMR, Xray analysis, electrochemistry, and photophysics. TD-DFT calculations were also undergone to rationalize the assignment of the photophysical properties. Some of these copper complexes exhibit very bright blue emission with high quantum yield at solid state. A variation of the electronic properties on both NHC and dipyridylamine ligands, has been carried out and permitted to establish a structure - properties relationship, also supported by TD-DFT calculations. A photophysical study at low temperature highlighted a specific luminescence phenomenon of the complexes: Thermally Activated Delayed Flurorescence. Since emissive cationic organometallic complexes can be good candidates for LEC (Light emitting Electrochemical Cells) applications, a selection of copper complexes was achieved for the preparation of those lighting devices. Here is presented the proof of concept that our copper complexes, of general formula [Cu(NHC)(dpa)][X], can be applied for LEC devices. To the best of our knowledge, we are presenting here the first blue emitting LEC device incorporating cationic copper complexes.⁽²⁾



Main body with references.^{1,2}

(1) Marion, R.; Sguerra, F.; Di Meo, F.; Sauvageot, E.; Lohier, J.-F.; Daniellou, R.; Renaud J.-L.; Linares, M.; Hamel, M. Gaillard, S. *Inorg. Chem.* **2014**, *53*, 9181-9191

(2) Elie, M.; Sguerra, F.; Di Meo, F.; Weber, M. D.; Marion, R.; Grimault, A.; Lohier, J.-F., Renaud, J.-L.; Costa, R. D.; Linares, M.; Hamel, M.; Gaillard, S. (Submitted)

[Cu <mark>Cl(NHC</mark>)]	<mark>dpa</mark> ligand EtOH, reflux, 1h	[Cu(NHC)(<mark>dpa</mark>)][PF₆] 56-98%	1) dpa ligand HBF₄·Et₂O	[Cu <mark>OH(NHC</mark>)]
	then K PF₆ aq.		toluene, r.t., 3h 2) KPF ₆ MeOH r.t. 1h	