

Phosphine tuning for heteroleptic $[\text{Cu}(\text{N}^{\wedge}\text{N})(\text{P}^{\wedge}\text{P})][\text{PF}_6]$ in light emitting electrochemical cells

F. Brunner¹, C. E. Housecroft^{1*}, E. C. Constable^{1*}

¹Department of Chemistry, University of Basel, Spitalstrasse 51, CH4056 Basel, Switzerland

Light emitting electrochemical cells (LEECs) are of growing importance in the field of flexible electronics and large surface lighting devices. Their simple device architecture, consisting of one emissive layer sandwiched between two electrodes (of which one has to be transparent) and the use of air stable materials make them fundamentally suitable for large area lighting as well as display applications. The emissive material usually consists of a semiconducting polymer or an emissive ion transition metal complex (iTMC) mixed with ionic liquid. Indium tin oxide (ITO) covered glass and aluminum are used readily as electrode materials. The emissive layer can be easily deposited by solution based methods such as spin coating, which makes the fabrication of a LEC fairly simple and less complex than the fabrication of e.g. an OLED (organic light emitting diode).

In the past iridium based transition metal complexes have been widely used in LECs. Their excellent colour tunability and the extremely long lifetime of the device of up to several thousand hours have led to the development of a wide range of iridium complexes for LEC applications. But the main drawback of iridium as a key compound is the low availability and the associated high costs of the material. Therefore scientists soon began to search for alternative metals for LEC applications. One very promising candidate was found to be copper. The high availability and low cost of this metal make it a suitable candidate for lighting applications.^[1]

Heteroleptic copper complexes of the type $[\text{Cu}(\text{N}^{\wedge}\text{N})(\text{P}^{\wedge}\text{P})][\text{PF}_6]$ where $\text{N}^{\wedge}\text{N}$ is a chelating diimine and $\text{P}^{\wedge}\text{P}$ is a chelating diphosphine ligand show strong emission upon excitation on an MLCT (metal-to-ligand charge transfer) level as well as in electroluminescence. The key aspect of these complexes is to sterically tune the copper coordination sphere to maintain the metal in a tetrahedral environment and shield it from access by small molecules such as solvents or oxygen. This preserves the copper in the oxidation state +I which is essential for the emissive nature of the compound.^[2]

In this work a series of new heteroleptic copper complexes is presented in which the phosphine ligand is tuned sterically and electronically to alter the emissive properties of the compound as well as the device functionality and lifetime.

[1] S. Tang and L. Edman, *Top. Curr. Chem.*, **2016**, 374, 1-21.

[2] S. Keller, A. Pertegás, G. Longo, L. Martínez, J. Cerdá, J. M. Junquera-Hernández, A. Prescimone, E. C. Constable, C. E. Housecroft, E. Ortí and H. J. Bolink, *J. Mater. Chem. C*, **2016**, 4, 3857-3871.