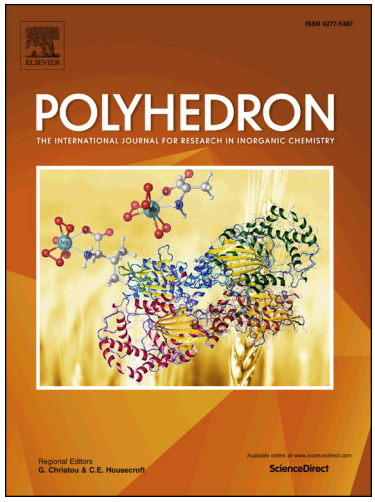

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PII: S0277-5387(17)30083-9
DOI: http://dx.doi.org/10.1016/j.poly.2017.01.046
Reference: POLY 12450

To appear in: *Polyhedron*

Received Date: 9 December 2016
Revised Date: 24 January 2017
Accepted Date: 25 January 2017

Please cite this article as: L-L. Hu, C. Shen, W-K. Chu, J. Xiang, F. Yu, G. Xiang, Y. Nie, C-L. Kwok, C-F. Leung, C-C. Ko, Synthesis, Structures and Photophysical Properties of Cu(I) Phosphine Complexes with Various Diimine Ligands, *Polyhedron* (2017), doi: http://dx.doi.org/10.1016/j.poly.2017.01.046

Synthesis, Structures and Photophysical Properties of Cu(I) Phosphine Complexes with Various Diimine Ligands

Lin-Li Hu,[a],† Chang Shen,[a],† Wing-Kin Chu,[b,c] Jing Xiang,[a],* Fei Yu,[a] Ge Xiang,[a] Yan Nie,[a] Chun-Leung Kwok,[d] Chi-Fai Leung,[d],* Chi-Chiu Ko*,[c]

[a] College of Chemistry and Environmental Engineering, Yangtze University, Jingzhou 434020, HuBei, P.R. China. Email: xiangjing@yangtzeu.edu.cn
[b] Faculty of Science and Technology, Technological and Higher Education Institute of Hong Kong, 20A Tsing Yi Road, Tsing Yi, Hong Kong, China
[c] Department of Biology and Chemistry, Institute of Molecular Functional Materials, City University of Hong Kong, Tat Chee Avenue, Kowloon Tong, Hong Kong, China. Email: vinccko@cityu.edu.hk
[d] Department of Science and Environmental Studies, The Education University of Hong Kong, 10 Lo Ping Road, Tai Po, Hong Kong, China. Email: cfleung@eduhk.hk
† These two authors contribute equally.

Abstract: A series of triphenylphosphine Cu(I) complexes with various diimine ligands, $[Cu(N\text{-}N)(PPh_3)_2](ClO_4)$ [N-N = **dmp** (**2**); **Ph_2Phen** (**3**); **Ph_2dmp** (**4**); **dpq** (**5**); **dppz** (**6**); **phenCN** (**7**); **phenOH** (**8**)] are synthesized by the ligand substitution reactions of $[Cu(MeCN)_4](ClO_4)$ with 2 mole equiv. of PPh_3 ligand and 1.2 mole equiv. of diimine ligand. {Cu(**dpq**)$[P(XPh)_3]_2$}(ClO_4) [X = Me (**5a**); OMe (**5b**); Cl (**5c**)] and {Cu(**phenOH**)$[P(XPh)_3]_2$}(ClO_4) [X = Me (**8a**); OMe (**8b**)] are also obtained by using various substituted phosphine ligands. These mixed-ligand complexes have been characterized using ^{1}H and ^{31}P NMR spectroscopy, IR spectroscopy, mass spectrometry and elemental analysis. Three of these complexes have been structurally characterized by X-ray crystallography. The photophysical and electrochemical properties of these complexes have been studied. These complexes exhibit MLCT phosphorescence with emission energy, lifetimes and quantum yields showing strong dependence on the nature of diimine and phosphine ligands. In particular, both the electronic and steric effects of the substituting groups in phosphine ligands are also found to affect the emission properties of the complexes. Our study provides structural-properties information for the future design of luminescent Cu(I) complexes.

Keywords: Luminescent properties; Cu(I) complexes; Crystal structures; Electrochemistry

Introduction

Phosphorescent complexes of noble metals, especially of iridium(III) and platinum(II) complexes, have been investigated extensively due to their extensive uses as emissive dopants in organic light-emitting diodes (OLEDs).[1] These phosphorescent materials are superior to fluorescent materials because they can harvest both singlet and triplet excitons in electroluminescence processes, leading to the high internal quantum efficiency.[2] These metals are, however, very expensive, since their earth abundance are rather limited.