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Cu(I) complexes regulated by N-heterocyclic ligands: syntheses, structures, fluorescence and electrochemical properties

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Abstract: Three mononuclear Cu(I) complexes, namely, $[Cu(2\text{-}PBO)(PPh_3)_2]\cdot ClO_4\cdot 2CH_2Cl_2$ (**1**), $[Cu(3\text{-}PBO)(PPh_3)_2(ClO_4)]\cdot CH_2Cl_2$ (**2**) and $[Cu(PBM)(PPh_3)_2]\cdot ClO_4$ (**3**) (2-PBO = 2-(2'-Pyridyl)benzoxazole, 3-PBO = 2-(3′-Pyridyl)benzoxazole, PBM = 2-(2′-Pyridyl)benzimidazole, PPh_3 = triphenylphosphine) have been synthesized and characterized by elemental analyses, IR, ^{1}H-NMR, ^{13}C-NMR, X-ray single crystal diffraction and thermal analysis. Photoluminescent investigation shows that complexes **1-3** exhibit distinct tunable light green (512nm)-to-yellow (557nm) photoluminescence by varying the N-heterocyclic ligands. Three complexes show intense 2-PBO-based yellow, 3-PBO-based light green and intense PBM-based bright green luminescence upon irradiation with a standard UV lamp (λ_{ex} = 254 nm) at room temperature. Moreover, the electrochemical properties of **1-3** have been investigated by cyclic voltammetry. The results suggest the frontier molecular orbits and the HOMO-LUMO energy gaps of these cuprous complexes are effectively adjusted through the introduction of different N-heterocyclic ligands, thus achieving the selective luminescence of the cuprous complexes.

Keywords: Copper(I) complex; Photoluminescent; Crystal structures; Electrochemical; N-heterocyclic

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