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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, $[\text{Cu}(\text{2-PBO})(\text{PPh}_3)_2]\cdot\text{ClO}_4\cdot 2\text{CH}_2\text{Cl}_2$ (**1**), $[\text{Cu}(\text{3-PBO})(\text{PPh}_3)_2(\text{ClO}_4)]\cdot\text{CH}_2\text{Cl}_2$ (**2**) and $[\text{Cu}(\text{PBM})(\text{PPh}_3)_2]\cdot\text{ClO}_4$ (**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, $^1\text{H-NMR}$, $^{13}\text{C-NMR}$, 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 ($\lambda_{\text{ex}} = 254 \text{ nm}$) 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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