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Synthesis, crystal structure, photoluminescence and theoretical studies of a series of copper(I) compounds based on imidazole derivatives

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ABSTRACT

Two mononuclear and one binuclear Cu(I) complexes that contain imidazole derivative ligands including 2-(2′-pyridyl)imidazole (L1), 2-(2′-pyridyl)benzimidazole(L2), and 2,6-bis (benzimidazol-2yl)-pyridine (L3) were synthesized. The formulas of these complexes are $[CuL1(PPh_3)_2][BF_4]$ (1), $[CuL2(PPh_3)_2][BF_4]$ (2), $[Cu_2(L3)_2(PPh_3)_2][BF_4]_2$ (3), respectively. The crystal structures of complexes 1–3 have been determined by single-crystal X-ray diffraction analyses. The Cu(I) ions in the complexes have a distorted tetrahedral geometry. Photophysical properties of complexes 1–3 were systematically studied. These complexes maximum emission are mainly concentrated in the 623–680 nm. An electroluminescent (EL) device using 2 as the emitter was fabricated. The device produced a red emission which matches with the PL spectrum. However, the EL device of 2 is unfavorable. The absorption properties of complexes 1 and 2 were theoretically analyzed by time-dependent density functional theory (DFT).The calculated results are in good agreement with the experimental data.

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1. Introduction

Phosphorescent materials based on heavy metal complexes have great potential applications, such as light-emitting devices, solar cells, or sensors/probes [1–7]. The phosphorescence compounds of the earlier studies focused on noble Ir(III), Pt-(II), and Ru(II)complexes [8–12]. In recent years, phosphorescent Cu(I) complexes receive much attention due to relatively abundant resource and nontoxic property, which make these complexes very applicable in solar energy conversion, biological probing, and organic light-emitting devices (OLEDs) [13–18]. Zn and Cd of imidazole complexes as Blue light emitting materials have been illustrated by our research groups [19,20]. However, Cu(I) of imidazole complexes has rarely been reported. A series of Cu(I) complexes with different phosphorous/phenanthroline ligands and their electro-luminescence (EL) performances have been reported by Wang and co-workers [21]. Li and co-workers reported electroluminescent colors can be tuned ranging from green-yellow to orange-red region using Cu(I) complexes as doped material [18]. Li and co-workers reported a series of Cu(I) complexes which exhibit a maximum brightness of 4483 cd/m^2 and a peak efficiency of 3.4 cd/A [22]. Heteroleptic Cu(I) complexes comprising imidazole derivatives and triphenylphosphine (PPh_3) are promising, because they are capable of producing MLCT phosphorescent emission [23,24]. In this work, we synthesized three novel Cu(I) complexes. We obtained the crystal structure of $[CuL1(PPh_3)_2][BF_4]_2$ (1), $[CuL2(PPh_3)_2][BF_4]_2$ (2), $[Cu_2(L3)_2(PPh_3)_2][BF_4]2$ (3). We reported the preparation, crystal structure, UV–Vis spectrum, fluorescence spectrum and DFT calculation of complexes.

2. Experimental

2.1. Materials and methods

Triphenylphosphine (referred as PPh_3), pyridine-2-aldehye and pyridine-2, 6-dicarboxylic acid were purchased from Aldrich and used without further purification. The other reagents and complexes were synthesized accord to procedures. UV–Vis spectrums of samples were recorded on a TU-1901 spectrometer. Fluorescence spectra of samples were recorded on a RF-5301 spectrometer. Elemental analyses were performed on a Perkin-Elmer 240c analyzer. ^{1}H NMR spectra of samples were recorded on a Brucker AC-80 spectrometer. IR spectra of samples were recorded on a MAGNA-560 spectrometer.

2.2. Synthesis of $[CuL1(PPh_3)_2][BF_4]$

2.2.1. Synthesis of $[CuL1(PPh_3)_2][BF_4]$ (1)

In 10 mL of dichloromethane, 0.525 g (0.002 mol) PPh_3 and 0.314 g (0.001 mol) $[Cu(CH_3CN)_4]BF_4$ were dissolved and was stirred for 1 h at room temperature. After a dichloromethane solution

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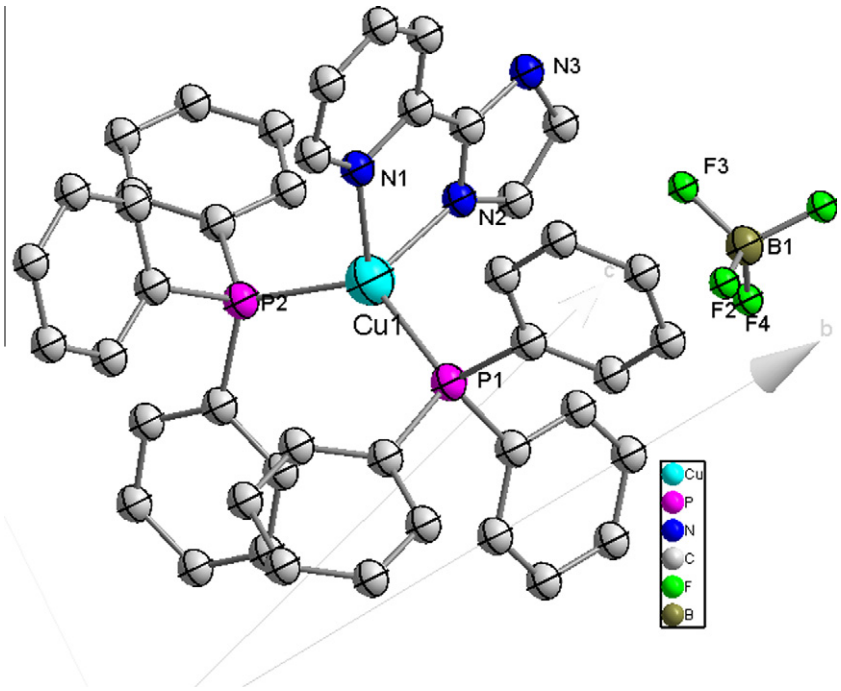

Fig. 1a. Molecule structure of complex 1.

(5 mL) of 0.135 g (0.001 mol) L1 was added, the solvent was stirred for another 4 h to give an orange solution. The solution was then filtered and evaporated to dryness. The residue was dissolved in dichloromethane and diffusion of methanol vapor into its concentrated solution gave orange crystals of 1 after 6 days (0.76 g, 78%). *Anal.* Calc. for $C_{44}H_{36}$ BCuF4N3OP2: C, 63.23; H, 4.31; N, 5.03. Found: C, 63.24; H,4.36; N, 5.05%. IR (cm^{-1}): IR (cm^{-1}): 1545, 1538, 1347, 765, 779. ^{1}H NMR (300 Hz, $CDCl_3$, 25 °C): δ 8.60(d, 2H, J = 8.0 Hz), 8.4 (d, 2H, J = 8.0 Hz), 8.01–7.75 (m, 20H), 7.51–7.36 (m, 12H). 31P NMR d + 1.71 (s).

2.3. Synthesis of [CuL2(PPh$_3$)$_2$][BF$_4$]

2.3.1. Synthesis of [CuL2(PPh$_3$)$_2$][BF$_4$] (2)

In 10 mL of dichloromethane, 0.525 g (0.002 mol) PPh_3 and 0.314 g (0.001 mol) $[Cu(CH_3CN)_4]BF_4$ were dissolved and was stirred for 1 h at room temperature. After a dichloromethane solution (5 mL) of 0.195 g (0.001 mol) L2 was added, the solvent was stirred for another 4 h to give an orange solution. The solution was then filtered and evaporated to dryness. The residue was dissolved in dichloromethane and diffusion of methanol vapor into its concentrated solution gave orange crystals of 2 after 7 days (0.77 g, 74%).

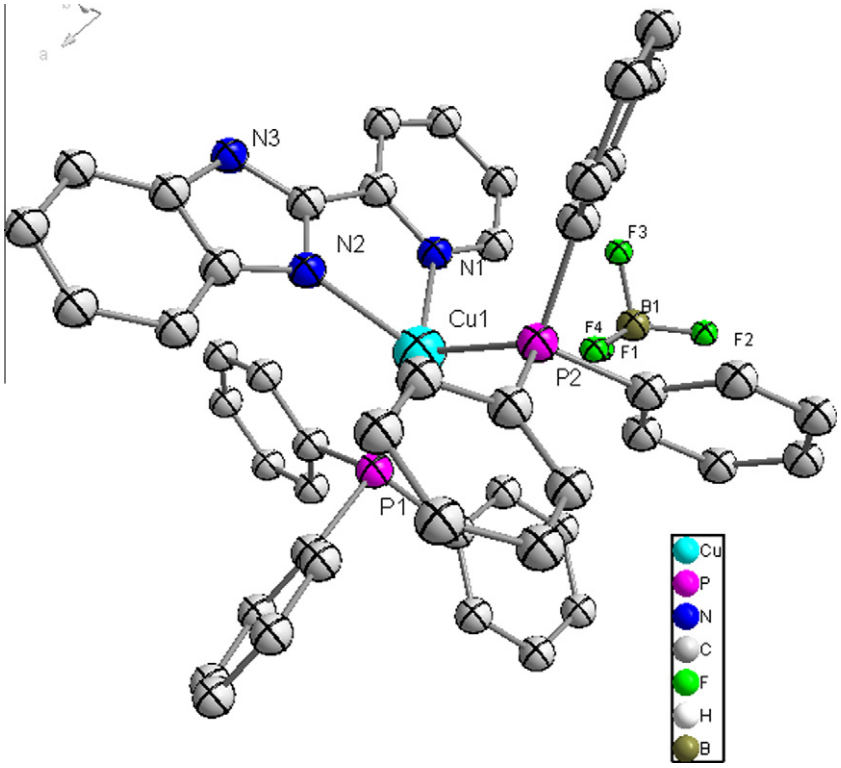

Fig. 1b. Molecule structure of complex 2.

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