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Research paper

Sev and pcu topological nets in one-pot newly synthesized mixed-ligand imidazole-containing Cu(II) coordination frameworks: Crystal structure, intermolecular interactions, theoretical calculations, magnetic behavior and biological activity

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ABSTRACT

Novel mixed-ligand coordination frameworks, occurring concomitantly namely $[Cu(Im)_3(H_2Cit)]$ (**1**) and $[Cu(Im)_2(HCit)]\cdot HIm$ (**2**) (with Im = imidazole and H_4Cit = citric acid) were obtained as a result of the one-pot reaction between imidazole, citric acid and copper chloride. The complexes were structurally characterized by elemental analysis, FTIR spectroscopy and X-ray diffraction. The two structures were found to be connected through 3D hydrogen-bonding networks examined by means of the *Hirshfeld* surface analysis which highlighted the presence of O–H···O, N–H···O and C–H···O H-bonds together with the $\pi\cdots lp$ interactions. A topological analysis of the underlying nets corresponding to the two hydrogen-bonded frameworks was carried out. Moreover, quantum chemical calculations were performed using the HF method with 6-31G(d) and LANL2DZ levels in the gas phase, and therefore the optimized structures, the IR, ^1H NMR, ^{13}C NMR spectra and the electronic structure descriptors were examined in detail. Furthermore, the magnetic properties of (**1**) and (**2**) were also investigated. The complexes showed remarkable antimicrobial and antifungal inhibition activities.

1. Introduction

The nitrogen atoms of the imidazole ring bear interesting physical and chemical properties that result in different pharmacological activities of the molecule and its derivatives [1]. Imidazole and its derivatives have been reported to have analgesic, anti-inflammatory, cardiovascular, anti-neoplastic, antifungal, enzyme inhibition, antiviral and antiulcer activities [2]. Moreover, the anti-parasitic and antiviral activities of aniline derivatives of imidazole have been described in the literature [3].

Imidazole occurs in most proteins as part of the side chain of histidine and constitutes a binding site for various transition metal ions in a large number of metalloproteins [4]. Consequently, the bonding between imidazole and transition metal ions is widely known [5] and of considerable interest especially in biological systems [6,7]. In order to understand the special magnetic and spectroscopic properties and the catalytic mechanisms of copper proteins, the study and modeling of the active site of copper-containing proteins has been a field of great interest within the scientific community [8]. Therefore, copper(II)–imidazole systems with different ratios of imidazole to copper have been prepared and investigated by several researchers [9]. Furthermore, being studied as models for copper proteins that contain both functionalities in the side chain [10], some mononuclear copper(II)–imidazole complexes with carboxylate ligands have been found to display a variety of pharmacological effects, including antitumor [11], superoxide dismutase and catecholase activities [12]. In particular, the recognition of the strong antitumor activity of the trans bis

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