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Experimental and *in silico* studies of dichloro-*tetrakis*(1H-pyrazole)-cobalt(II): Structural description, photoluminescent behavior and molecular docking

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ABSTRACT

A novel pyrazole-based Co(II) complex, namely dichloro-tetrakis(1H-pyrazole)-cobalt(II), was synthesized and characterized. Its X-ray crystal structure showed that it crystallizes in the monoclinic *C*2/*c* space group with discrete $[CoPz_4Cl_2]$ units held together *via* intra- and intermolecular hydrogen bonds. The non-covalent interactions were explicitly analyzed by means of the topological and *Hirshfeld* surface analyses, revealing the presence of 0-periodic binodal 1,6-connected **1,6M7–1** and 14-connected uninodal **bcu–x** topologies built up through N—H…Cl and C—H…Cl hydrogen-bonding networks in addition to weak non-classical H…H, N–H…C, C–H…N, N—H…π, π…*lp*/*lp*…π and *lp*…*lp* interactions. Additionally, interactions energy and energy frameworks analyses were performed in order to compute the total energies of the possible intermolecular interactions. The empty space in the crystal lattice was analyzed using *void mapping* which lead to the presence of small cavities. The structure was furthermore optimized showing a very good agreement with the experimental results, the molecular electrostatic potential (MEP) maps were obtained with their active regions and the non-linear optical properties estimated. Additionally, the optical properties of the title complex were investigated at room temperature using optical UV-visible absorption and photoluminescence spectroscopy, exhibiting $\pi \rightarrow \pi^*$, n $\rightarrow \pi^*$, $d \rightarrow d$ and ligand-field transitions which result in a large variety of emission bands predominant by a bright red photoluminescence. An *in silico* study was carried out and the binding ability of the title complex with *Staphylococcus aureus* tyrosyl-tRNA synthetase and *Pyrococcus kodakaraensis* aspartyl-tRNA synthetase was evaluated displaying a good inhibition activity towards the last one.

1. Introduction

Heterocyclic compounds containing nitrogen, oxygen and sulfur, and their metal complexes are biologically active materials toward bacteria, fungi and viruses [1–5]. Especially, pyrazole-based ones, referred to hereafter as Pz, are applied in the pharmaceutical and agrochemical fields [6]. The pyrazolate ligand can exhibit three coordination modes. It can act as a monodentate (pyrazole-N) and exo-bidentate (pyrazole N,N) or an endo-bidentate ligand [7,8]. In most cases, the pyrazolate ligand coordinates in an exo-bidentate fashion, thus linking two metal centres that may be identical or different. Recent studies have described the catalytic activity of pyrazolate complexes [8,9] under mild conditions, thus encouraging the exploration of these ligands.

In fact, since the first review of pyrazole-derived ligands appeared in 1972 [10], the coordination chemistry of Pz and its derivatives has strongly evolved over the last two decades [11]. Pz derivatives have many other applications such as analgesic [12], antibacterial [13], anti-hyperglycemic [14], anti-inflammatory [15], antipyretic [16], hypoglycaemic [17] and sedative hypnotic activities [18]. The ones such as *celecoxib, rimonabant, fomepizole* and *sildenafil* were established as selective drugs [19]. In fact, *celecoxib* demonstrated anti-inflammatory effect and inhibited cox-2 [20], while *rimonabant* is a cannabixiod receptor and is used for obesity treatment. *Bindenafil* and *fomepizole* inhibit phosphodiesterase

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