Journal of the Iranian Chemical Society (2020) 17:671–685
https://doi.org/10.1007/s13738-019-01805-0

ORIGINAL PAPER

Crystal structure, *Hirshfeld* surface analysis and theoretical calculations of an oxalato-bridged copper(II) complex: *μ*-oxalato-bis[(2,2′-bipyridine) hydrate copper(II) nitrate]

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Received: 7 December 2018 / Accepted: 25 October 2019 / Published online: 5 November 2019

Abstract

The copper complex $[Cu_2(Bipy)_2(H_2O)_2(C_2O_4)(NO_3)_2]$ (Bipy = 2,2′-bipyridine; $C_2O_4^{2-}$ = oxalate) has been synthesized and characterized by single-crystal X-ray diffraction and FTIR spectroscopy. The structure determination revealed that the title compound contains centrosymmetric doubly charged dinuclear oxalato-bridged copper(II) complex cations, nitrate counter ions and water molecules. In this complex, the oxalate ligand is coordinated in a bis-bidentate bridging mode to the copper atoms. Each Cu(II) atom has a distorted tetragonal–bipyramidal environment, being coordinated by two N atoms of a chelating 2,2′-bipyridine ligand and two O atoms of the doubly deprotonated oxalate anion. Pairs of monodentate nitrate anions and aqua ligands are linked to the metallic cations in an axial position. The H-bonds occurring in the crystal structure result in the formation of 2D supramolecular chains and 3D networks. The *Hirshfeld* surface analysis of the complex has shown the presence of strong O–H…O and C–H…O hydrogen bonds together with non-classical weak C–H…*π*, *π*…*π*, *π*…*lp*/*lp*…*π* and *lp* …*lp* interactions. Furthermore, the theoretical calculations results are in agreement with the experimental geometric parameters. The NMR spectra and the MEP maps were also calculated.

Keywords Oxalato-bridged complexes · Crystal structure · Hydrogen bonds · *Hirshfeld* surface analysis · Theoretical calculation · MEP

Introduction

The ability of the oxalate anion to generate di- and polynuclear complexes is well known. The rich structural diversity of the oxalato-bridged complexes is due to the exceptional versatility of the oxalate ligand. Moreover, the oxalate bridge can efficiently mediate the exchange interactions between the paramagnetic metal ions, leading to interesting magnetic properties [1–4]. The magnetic interactions through the bridge depend markedly upon the coordinated ligands and the counter ions [5]. A great number of oxalato-bridged dinuclear complexes have been characterized so far [5–10]. These compounds are generally obtained through the reaction between a cationic complex having potentially free coordination sites and the oxalate anion. The construction of oxalate-containing homo- and hetero-metallics, which have applications as molecular-based magnetic materials, has enhanced the interest in the oxalato compounds.

We report herein the synthesis, the crystal structure and the computational studies, accomplished using the

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