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Abstract

Interactions Energy, Energy Frameworks, *Hirshfeld* Surface and Topological Analyses of a Mononuclear Co(II) Coordination Framework †

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Heterocyclic ligands and their metallic complexes are biologically active materials [1–5], especially pyrazole-based ones, which are used in the pharmaceutical and agrochemical fields [6]. Accordingly, pyrazole-based copper and cobalt complexes showed excellent antibacterial and antifungal activities [7–9]. Particularly, the copper complexes were reported to have biological properties and some of them were active both in vivo and in vitro [9,10]. On the other hand, many stable [M(Hpyrazole)$_4$X$_2$] complexes resulting from several transition metal cations with pyrazole and substituted-pyrazoles were reported [11–16]. In order to contribute to this complexes' family, a Co(II) complex, namely dichloro-tetrakis(1H-pyrazole)-cobalt(II) [17], was synthesized and structurally characterized by means of single-crystal X-ray diffraction. The hydrogen bonds and the non-covalent interactions within the complex were explicitly analyzed by means of the *Hirshfeld* surface analysis which showed the presence of 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. The hydrogen-bonds and the non-covalent interactions within the complex were explicitly analyzed by means of the *Hirshfeld* surface analysis [18] which showed the presence of 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, the interactions energy and energy frameworks analyses [19] were performed in order to compute the total energies of the possible intermolecular interactions. The empty space in the crystal lattice was also analyzed using *void mapping* which lead to the presence of small cavities. The structure was furthermore examined by means of the topological analysis [20], which revealed the presence of 0-periodic binodal 1,6-connected **1,6M7-1** and 14-connected uninodal **bcu-x** [21] topologies.

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Data Availability Statement: Full structural details might be found in the CIF file deposited at the Cambridge Crystallographic Data Centre, CCDC No 2032295. This data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html, or from the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK; Fax: +44-01223-336-033; e-mail: deposit@ccdc.cam.ac.

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