Metal-organic frameworks (MOFs) consist of metal ions or clusters often coordinated to rigid organic molecules to form one-, two-, or three-dimensional structures. Pyrazole ligands have been widely used in order to build new MOFs and their properties and applications have been extensively investigated [1-3]. Furthermore, the pyrazole derivatives have been widely used to design materials and complexes with interesting hydrogen bonding interactions. The pyrazole based complex : trans-Dichlorotetrakis(1H-pyrazole-κN2)copper(II) has been structurally characterized by means of FT-IR, Raman spectroscopies and single-crystals X-rays diffraction. It’s noteworthy that the crystal structure of this complex has been mentioned three times in the earlier literature [4-7]. However, its vibrational, structural DFT study [8], magnetic properties and antimicrobial activity have been investigated for the first time. Moreover, the Hirshfeld surfaces used to define the intermolecular environment of the molecules within the crystal together with the 2D-fingerprint graphics allowing exploring the properties and the occurrence of each intermolecular contact in the studied complex will be discussed in detail and compared to other similar derivatives.


Keywords: MOFs, DFT calculation, Magnetic and antimicrobial properties