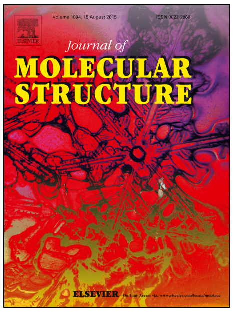

A Hirshfeld surface analysis, supramolecular structure and magnetic properties of a new Cu(II) complex with the 4-amino-6-methoxypyrimidine ligand

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A Hirshfeld Surface Analysis, supramolecular structure and magnetic properties of a new Cu(II) complex with the 4-amino-6-methoxypyrimidine ligand

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Abstract

A new Cu(II) complex with the bridge bidentate ligand 4-amino-6-methoxypyrimidine, $[Cu(C_5H_7N_3O)(H_2O)(NO_3)_2]$, has been prepared at room temperature and characterized by single crystal X-ray diffraction and IR spectroscopy. The compound crystallizes in the monoclinic space group C2/c with lattice parameters a = 17.783 (4), b = 11.131 (3), c =12.594 (3) Å, β = 117.616 (3)°, V = 2209.0 (9) Å^3 and Z = 8. The Cu(II) cation is hexa-coordinated, in distorted octahedral fashion, by two nitrogen atoms of two 4-amino-6-methoxypyrimidine ligands, one water oxygen atom and three oxygen atoms of two nitrate anions. In the atomic arrangement, the organic ligands and the 6-connected Cu centers are linked with each other to give a 1-D corrugated chain running along the b-axis direction. The chains are interconnected via O—H···O, C—H···O, N—H··O hydrogen bonds to form a three dimensional network. The analysis of contacts on the Hirshfeld surface shows that the crystal packing is driven mainly by the electrostatic interactions: the coordination of Cu(II) by