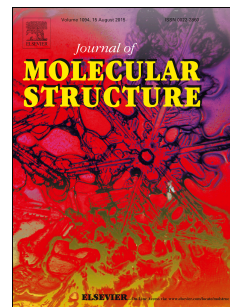


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# A Hirshfeld Surface Analysis, supramolecular structure and magnetic properties of a new Cu(II) complex with the 4-amino-6-methoxypyrimidine ligand

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## Abstract

A new Cu(II) complex with the bridge bidentate ligand 4-amino-6-methoxypyrimidine,  $[\text{Cu}(\text{C}_5\text{H}_7\text{N}_3\text{O})(\text{H}_2\text{O})(\text{NO}_3)_2]$ , 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,  $\beta = 117.616(3)^\circ$ ,  $V = 2209.0(9)$  Å<sup>3</sup> 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  $\text{O}—\text{H}\cdots\text{O}$ ,  $\text{C}—\text{H}\cdots\text{O}$ ,  $\text{N}—\text{H}\cdots\text{O}$  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

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