Crystal and geometry-optimized structure, Hirshfeld surface analysis and physicochemical studies of a new Co(II) complex with the ligand 2-amino-6-methoxypyrimidine.

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The crystal structure of the new complex [Co(C5H7N3O)2(H2O)4](NO3)2·4H2O synthesized in aqueous solution has been determined by single crystal X-ray diffraction. The compound crystallizes in the triclinic space group P with lattice parameters: a = 7.3056(2), b = 8.4065(2), c = 10.4724(3) Å, α = 103.9470(19), β = 105.6600(14), γ = 91.1350(18)°, V = 598.54(3) Å3 and Z = 1. The Co(II) central ion is in a slightly distorted octahedral coordination geometry formed by two nitrogen atoms of two 2-amino-6-methoxypyrimidine ligands and four oxygen atoms of coordinated water molecules. The crystal packing is stabilized by intermolecular OH···O, NH···O and CH···O hydrogen bonds which link the molecules into a three-dimensional network. Intermolecular interactions were investigated by Hirshfeld surfaces. Electronic properties such as HOMO and LUMO energies were derived. The vibrational absorption bands were identified by infrared spectroscopy. The compound was characterized by thermal analysis to determine its thermal behavior with respect to temperature.

Słowa kluczowe

Coordination compound, X-ray diffraction, Hirshfeld surface, Contact enrichment ratio, DFT calculations

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