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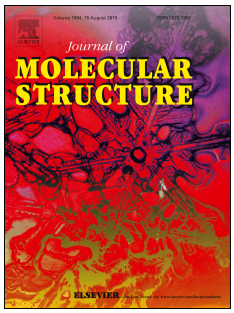

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Synthesis, crystal structure, physico-chemical characterization of a new hybrid material, (2-hydroxyethyl)piperazine-1,4-diium hexachlorostannate(IV) monohydrate

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Abstract

The new organic-inorganic compound $[C_6H_{16}N_2O](SnCl_6).H_2O$ was synthesized and single crystals were grown from an aqueous solution through these slow evaporation technique. The atomic arrangement can be described by organic-inorganic layers parallel to the (a, c) plane. These layers are connected via hydrogen bonds (O-H…O and C-H…Cl) to build a three dimensional arrangement. The ^{13}C and ^{15}N CP-MAS NMR spectra are in agreement with the X-ray structure. The vibrational absorption bands were identified by infrared spectroscopy and Raman scattering. DFT calculations allowed the attribution of the IR bands. The 3D Hirshfeld surfaces and the associated 2D fingerprint plots were investigated for intermolecular interactions. X-ray photoelectron spectroscopy analysis (XPS) is a technique for analyzing the surface chemistry of a compound. It was employed to measure the elemental composition and electronic state of the elements within a material. The DSC profile shows endothermic peaks centered at approximately 343, 370 and 552 K.

Keywords: Organic-inorganic hybrid; X-ray diffraction; DFT calculations; spectroscopy; Hirshfeld surface, XPS.

1. Introduction