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Experimental and DFT characterization of the organic-inorganic monohydrated Co(II) complex with 2,6-diaminopyridine ligand, $(C_5H_8N_3)_2[CoBr_4]\cdot H_2O$.

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Streszczenie

Single crystals of the new organic-inorganic compound (C5H8N3)(2)[CoBr4]center dot H2O were grown by hydrothermal technique and characterized by X-ray diffraction, infrared absorption, raman spectroscopy scattering, optical absorption and thermal analysis. The title compound belongs to the triclinic space group PT and in the crystal structure, the inorganic layers are built from tetrabromidocobaltate anions [CoBr4](2-) and free water molecules, linked together by O-H center dot center dot center dot Br hydrogen bonds and halogen...halogen interactions. The organic cations are intercalated between the mineral layers via N-H center dot center dot center dot Br hydrogen bonds and form chains through 7C.iv interactions. Theoretical calculations were performed using density functional theory with the B3LYP/LanL2DZ level for studying the molecular structure and vibrational spectra of the title compound. Good consistency is found between the calculated results and the experimental structure, IR and Raman spectra. The optical properties were investigated by optical absorption showing Ligand-to-Metal Charge-Transfer transitions in the visible region and organic related it-it transitions in the UV region.

Słowa kluczowe

x-ray diffraction, Metal halides, density functional calculations, Optical absorption and thermal studies

Adres publiczny

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