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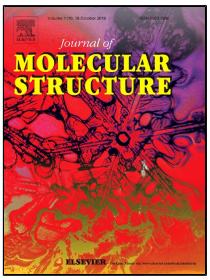

Crystal structure, vibrational studies and optical properties of a new organic phosphate $(C_{12}H_{14}N_2S)(H_2PO_4)_2$

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Crystal structure, vibrational studies and optical properties of a new organic phosphate $(C_{12}H_{14}N_2S)(H_2PO_4)_2$

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Abstract

The present work is atone for experimental study of crystal structure, vibrational spectra, thermal study and optical characterization of a new organic inorganic hybrid compound. This new material, $(C_{12}H_{14}N_2S)(H_2PO_4)_2$, was prepared by slow evaporation at room temperature. $(C_{12}H_{14}N_2S)(H_2PO_4)_2$ crystallize in the monoclinic space group C2/c. The structural resolution shows the existence of $H_2PO_4^{2-}$ anions liked together, via O-H…O hydrogen bonds, forming two-dimensional sheets parallel to (001) plane. These sheets are built of two types of rings. The 2,2'-diammonium-diphenyl sulfide cations are linked to these sheets by means of multiple N-H…O hydrogen bonds forming a three-dimensional net-work. ^{13}C NMR study was conducted for the grown crystal. Functional groups present in the compound were identified by IR and Raman spectral studies. TGA and DSC analysis were carried out to study the thermal behavior of the prepared material. The optical study was investigated by UV-Vis absorption. The spectrum shows the existence of two types of transitions. The optical band gap is determined to be 4.96 eV confirming the large transmittance of these crystals in the visible range of the spectrum.

KEY WORDS: Organic-inorganic phosphate, Hydrogen bonds, Crystal structure, Thermal analysis, optical characterization.