Crystal structure, Hirshfeld surface analysis, thermal behavior and spectroscopic investigations (FT-IR and CP-MAS NMR)) of a new organosulfate, $[C_6H_{22}N_4]^{4+}(SO_4^{2-})(HSO_4^{-})_2$

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Streszczenie

Crystals of a new organosulfate, $[C_6H_{22}N_4]^{4+}(SO_4^{2-})(HSO_4^{-})_2$ **I** were prepared at room temperature by slow evaporation. Suitable crystals have been subjected to X-ray diffraction, TG-DTA, IR and NMR spectroscopy accomplished with DFT calculation. The results of these investigations are discussed. The combination of N,N'-Bis(2-aminoethyl)ethane-1,2-diamine with sulfuric acid was confirmed by FT-IR studies using a Nicolet IR200 FT-IR spectrometer in the range 4000-400 cm^{-1}. The crystal data of the title compound were collected by subjecting the grown samples to single crystal XRD and the study reveals that the organosulfate is triclinic and it belongs to P space group. The calculated lattice parameter values are a = 9.3851(2), b = 11.5963(3), c = 16.2294(4) Å, α = 102.0600(10), β = 101.4790(10), γ = 98.8180(10) °, Z = 4 and V = 1657.39(7) $Å^3$. From the structural investigation, it is found that the studied compound is built by trimers resulting from the association of SO_4^{2-} and HSO_4^{-} anions through O-H…O hydrogen bonds to form rows propagating along the b direction. The tetracations connect these rows via N-H...O hydrogen bonds and C-H...O interactions to create a three-dimensional framework. From the infrared spectroscopy analysis, the functional groups were identified. Simultaneously, the thermal behavior, NMR spectroscopy and Hirshfeld surface analyses were also elucidated.

Słowa kluczowe

X-ray diffraction, Thermal behavior, CP-MAS NMR, Hirshfeld surface, DFT

Adres publiczny

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