Crystal Structure, Vibrational Spectrum and Thermal Behavior of the Ammonium Hexathiohypodiphosphate Dihydrate, $(NH_4)_4P_2S_6 \cdot 2\,H_2O$

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Single crystals of $(NH_4)_4P_2S_6 \cdot 2\,H_2O$ could be obtained and the crystal structure determined (monoclinic, $P2_1/c$ with $a = 6.931(1)$, $b = 12.730(2)$, $c = 17.446(2)$ Å, $\beta = 96.87(1)^\circ$, $V = 1528.2(4)$ Å^3, $Z = 4$). The NH_4^+, and $[P_2S_6]^{4-}$ ions and the water molecules are involved in an extended hydrogen-bonding network. The FT-Raman and FT-IR spectra have been recorded and the observed vibrational frequencies assigned to tetrahedral NH_4^+ and $[P_2S_6]^{4-}$ (D_{3d}) ions as well as to H_2O molecules. The thermogravimetric analysis has shown that $(NH_4)_4P_2S_6 \cdot 2\,H_2O$ starts to decompose at around 60 °C (up to 170 °C), but no distinct intermediates could be observed.

Key words: Hexathiodiphosphate(IV), Hexathiohypodiphosphate, Crystal Structure, Raman, IR