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Structure and vibrational spectra of $Na_5H_3(SeO_4)_4 \cdot 2H_2O$ crystal.

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Streszczenie

Pentasodium trihydrogen tetraselenate dihydrate crystals, $Na_5H_3(SeO_4)_4 \cdot 2H_2O$, are triclinic, space group P with a=5.959(3), b=7.268(4), c=9.958(4) Å, α = 102.50(3), β = 98.71(4), γ = 100.36(4)° and Z = 1. The crystal structure is determined from three-dimensional X-ray diffraction data taken on an automatic diffractometer with Mo $K\alpha$ radiation, and refined by least-squares techniques to R = 0.0295 for 2497 non-zero reflections. Two selenate ions from hydrogendiselenate anion by means of a short centrosymmetric O···O hydrogen bond of length 2.476(4) Å. Two crystallographically equivalent hydrogenselenate ions are linked to the hydrogendiselenate through the hydrogen bonds with the O···O distance of 2.592(4) Å. Trihydrogen tetraselenate moieties thus formed are joined into chains along the [111] direction via water molecules which form hydrogen bonds (2.859(4) and 2.767(5) Å) with the O(4) atoms of two adjacent unit cells. Powder IR and Raman spectra of the title crystal and its deuterated analogue have been measured. Two bands at 2850 and 2475 cm^{-1} are assigned to the stretching vibrations of the O(5)-H···O(3) hydrogen bonds. The broad band at ca. 1330 cm^{-1} and a background in the low frequency part of a spectrum are assigned to the stretching vibrations of the short O(1)···O(I^i) hydrogen bonds. An assignment of the internal vibrations of the selenate groups is proposed.

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