

Structure and vibrational spectra of  $\text{Na}_5\text{H}_3(\text{SeO}_4)_4 \cdot 2\text{H}_2\text{O}$  crystal.

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## Streszczenie

Pentasodium trihydrogen tetraselenate dihydrate crystals,  $\text{Na}_5\text{H}_3(\text{SeO}_4)_4 \cdot 2\text{H}_2\text{O}$ , are triclinic, space group  $P$  with  $a=5.959(3)$ ,  $b=7.268(4)$ ,  $c=9.958(4)$  Å,  $\alpha = 102.50(3)$ ,  $\beta = 98.71(4)$ ,  $\gamma = 100.36(4)^\circ$  and  $Z = 1$ . The crystal structure is determined from three-dimensional X-ray diffraction data taken on an automatic diffractometer with  $\text{Mo K}\alpha$  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  $\text{O}\cdots\text{O}$  hydrogen bond of length  $2.476(4)$  Å. Two crystallographically equivalent hydrogenselenate ions are linked to the hydrogendiselenate through the hydrogen bonds with the  $\text{O}\cdots\text{O}$  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  $\text{O}(4)$  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  $2475\text{ cm}^{-1}$  are assigned to the stretching vibrations of the  $\text{O}(5)\text{-H}\cdots\text{O}(3)$  hydrogen bonds. The broad band at ca.  $1330\text{ cm}^{-1}$  and a background in the low frequency part of a spectrum are assigned to the stretching vibrations of the short  $\text{O}(1)\cdots\text{O}(\text{I}')$  hydrogen bonds. An assignment of the internal vibrations of the selenate groups is proposed.

## Adres publiczny

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