

## Single-crystal FTIR and X-ray study of vishnevite, ideally $[\text{Na}_6(\text{SO}_4)][\text{Na}_2(\text{H}_2\text{O})_2](\text{Si}_6\text{Al}_6\text{O}_{24})$

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### ABSTRACT

This paper reports a single-crystal FTIR spectroscopic study of vishnevite, ideally  $[\text{Na}_6(\text{SO}_4)[\text{Na}_2(\text{H}_2\text{O})_2](\text{Si}_6\text{Al}_6\text{O}_{24})$ , a member of the cancrinite group of feldspathoids. The study was done on several crystals from various geological occurrences. Infrared spectra show that most samples, and in particular the specimens from the holotype locality at Vishnevye Mountains (Urals, Russia), contain molecular  $\text{CO}_2$  as the main carbon species in the structural pores, while the specimens from Loch Borolan (Scotland) were found to be  $\text{CO}_3$ -rich. Polarized-light measurements show that the linear  $\text{CO}_2$  molecules are oriented perpendicular to the crystallographic  $c$  axis. Structure refinement of sample Pi4 from Latium (Italy) shows usual  $\text{H}_2\text{O}\cdots\text{Na}\cdots\text{H}_2\text{O}$  sequences within the undecahedral cages; however, difference Fourier maps suggest the presence of additional protons in the channels, possibly forming OH groups. The FTIR spectra show three absorptions in the  $3800\text{--}3200\text{ cm}^{-1}$  region. The first one, at  $3590\text{ cm}^{-1}$  is strongly polarized for  $\text{E}_{\perp}c$  while the second, at  $3535\text{ cm}^{-1}$ , behaves almost isotropic. These two bands are assigned to the stretching vibrations of an asymmetric water molecule in the structural cages. The third broad absorption at  $3320\text{ cm}^{-1}$ , is predominantly polarized for  $\text{E}_{\parallel}c$  and is assigned to additional OH groups in the channels. Detailed microspectroscopic mapping showed several samples from Latium (Italy) to be zoned with respect to the  $\text{CO}_2/\text{CO}_3$  content, thus pointing to a possible use of the volatile content of these minerals for petrological modeling.

**Keywords:** Vishnevite, EMPA, crystal structure refinement, FTIR spectroscopy, channel molecules