Fourier Transform Infrared and Raman Spectra of Hexagonal $MgCsPO_4 \cdot 6H_2O$

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The Fourier transform infrared and Raman spectra of a struvite analogue, hexagonal magnesium caesium phosphate hexahydrate, $MgCsPO_4 \cdot 6H_2O$ and of its partially deuterated analogues were recorded from room temperature (RT) down to the boiling temperature of liquid nitrogen (LNT).

The crystal structure of hexagonal $MgCsPO_4 \cdot 6H_2O$ has been solved by X-ray diffraction [1]. According to the crystallographic results, it crystallizes in the hexagonal space group $P6_3mc$ (C_{6v}^4) with $Z = 2$. It was found that Mg^{2+}, Cs^+ and PO_4^{3-} occupy special positions with C_{3v} symmetry, while the two types of water molecules are situated on positions with C_s symmetry.

The existence of strong hydrogen bonds formed by the water molecules is supported by the appearance of a broad band from 3600 to 2200 cm^{-1} in the O–H stretching region of the vibrational spectra. In the difference LNT infrared spectrum of the analogue with a small deuterium content (≈ 5 % D), in the region of the OD stretching vibrations of isotopically isolated HDO molecules, at least two bands (from the expected three) at 2255 and 2180 cm^{-1} are observed.

In the infrared region of the $\nu_3(PO_4)$ modes, a broad and asymmetric band at around 1000 cm^{-1} is found, while in the region of the $\nu_4(PO_4)$ bending vibrations and of the external modes of the water molecules, several bands can be seen. The intense band at 945 cm^{-1} in the Raman spectra can be attributed with certainty to the components of the $\nu_1(PO_4)$ mode. On the basis of a careful analysis of the RT and LNT spectra of the protiated compound, as well as those of its partially deuterated analogues, the asymmetric band at around 550 cm^{-1} was assigned to the $\nu_4(PO_4)$ modes, the bands between 470 and 430 cm^{-1} to the $\nu_2(PO_4)$ vibrations and the remaining ones to librational and translational modes of the water molecules.

[1] A. Ferrari, L. Cavalca, M. Nardelli, *Gazz. Chim. Ital.* 85 (1955) 1232.