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VIBRATIONAL SPECTRA OF MAGNESIUM HYDROGENPHOSPHATE TRIHYDRATE AND OF ITS MANGANESE ANALOGUE

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Abstract The infrared (IR) and Raman spectra of $MgHPO_4 \cdot 3H_2O$ and of a series of partially deuterated analogues as well as the IR spectra of $MnHPO_4 \cdot 3H_2O$ have been recorded and interpreted. The analysis of the IR spectra in the HOD bending region rules out the possibility of existence of H_3O^+ ions in the structure.

Key Words: Infrared spectra, Raman spectra, magnesium hydrogenphosphate trihydrate, manganese hydrogenphosphate trihydrate, newberyite, deuterated analogues.

Recorded and interpreted were the infrared (IR) spectra of $MgHPO_4 \cdot 3H_2O$ (newberyite) and $MnHPO_4 \cdot 3H_2O$. Also recorded were the IR spectra of a series of deuterated analogues of newberyite and the Raman spectra of $MgHPO_4 \cdot 3H_2O$ and its fully deuterated analogue. The close resemblance of the IR spectra of $MgHPO_4 \cdot 3H_2O$ and $MnHPO_4 \cdot 3H_2O$ is not surprising since the two title compounds are isomorphous [1,2].

Of the Raman bands present in the ν(PO) region, three are due to modes localized in the PO_3 fragment (they are found above 950 cm^{-1}), whereas the P–O(H) stretch gives rise to the band around 892 cm^{-1} which on deuteration shifts to 877 cm^{-1}. In the IR spectrum the assignment is more difficult since the corresponding band is overlapped with the γ(P–O–H) one. The analogue of the latter band in the spectrum of the deuterated newberyite is found around 650 cm^{-1}.

The appearance of the IR bands at approximately 2200 and 2400 cm^{-1} is in line with the appreciable strength of the hydrogen bonds formed by the HPO_4^{2-} ions [1]. The presence of chains of such bonds shows that the two studied compounds are potential proton conductors. In the IR spectra of the partially deuterated analogues, bands due to δ(HOD) modes are present with shapes practically identical to those of the corresponding HOH ones. The presence of these bands definitely rules out the suspected [3] possibility of existence of H_3O^+ ions in the structure of the studied compounds since in the latter case bands due to the H_2DO^+ and HD_2O^+ species would be present.

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