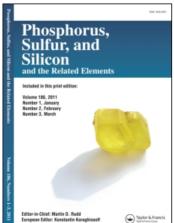
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Bojan Šoptrajanov^a; Gligor Jovanovski^a; Viktor Stefov^a; Igor Kuzmanovski^a
^a Institut za hemija, PMF, Univemitet "Sv. Kiril i Metodij", Skopje, Republic of Macedonia

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VIBRATIONAL SPECTRA OF MAGNESIUM HYDROGENPHOSPHATE TRIHYDRATE AND OF ITS MANGANESE ANALOGUE

BOJAN ŠOPTRAJANOV, GLIGOR JOVANOVSKI, VIKTOR STEFOV AND IGOR KUZMANOVSKI

Institut za hemija, PMF, Univerzitet "Sv. Kiril i Metodij", PO Box 162, 91001 Skopje, Republic of Macedonia

Abstract The infrared (IR) and Raman spectra of MgHPO₄ · $3H_2O$ and of a series of partially deuterated analogues as well as the IR spectra of MnHPO₄ · $3H_2O$ 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 MgHPO₄ · $3H_2O$ (newberyite) and MnHPO₄ · $3H_2O$. Also recorded were the IR spectra of a series of deuterated analogues of newberyite and the Raman spectra of MgHPO₄ · $3H_2O$ and its fully deuterated analogue. The close resemblance of the IR spectra of MgHPO₄ · $3H_2O$ and MnHPO₄ · $3H_2O$ is not surprising since the two title compounds are isomorphous [1,2].

Of the Raman bands present in the $\nu(PO)$ 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 $\gamma(P-O-H)$ 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 HPO₄²⁻ 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 $\delta(\text{HOD})$ 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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