



Vibrational spectroscopic study of hydroxypyromorphite-hydroxylmimetite solid solutions

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Hydroxypyromorphite $\text{Pb}_5(\text{PO}_4)_3\text{OH}$ and hydroxylmimetite $\text{Pb}_5(\text{AsO}_4)_3\text{OH}$ minerals belong to the apatite supergroup. Their structure allows isomorphous substitutions in both cationic and anionic positions. They are isostructural with pyromorphite $\text{Pb}_5(\text{PO}_4)_3\text{Cl}$ and mimetite $\text{Pb}_5(\text{AsO}_4)_3\text{OH}$ which are the end products of in situ phosphate induced remediation of soils polluted with heavy metals e.g. lead. The research objective was to synthesize and characterize the members of above mentioned solid solution. The minerals were synthesized at room temperature and analyzed by X-Ray diffraction and Infrared spectroscopy (FTIR-DRIFT).

The product syntheses was crystalline phase without any impurities within the detection limit of XRD. Shifts of certain diffraction peaks were observed in solid solution series due to replacement PO_4 after AsO_4 .

The bands ν_3 and ν_4 attributed to vibrations in the PO_4 and AsO_4 tetrahedra appear at 1050-790 and 580-534 cm^{-1} . Due to difference in atomic mass of P and As as well as bonding strength of P-O and As-O the skeletal bands shift to lower wavenumbers with the increase of AsO_4 substitution.

The correlation between the position of vibrational modes and the chemical composition is observed. The OH stretching mode in the FTIR spectra appears in the range of 3765-3552 cm^{-1} as a sharp band for the end members of the solid solution. For the intermediate minerals the OH band becomes complex. The analysis of deconvoluted OH bands indicated several vibrational modes which suggested a significant change of OH group local environment induced by substitutions.

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