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X-ray and neutron Rietveld refinement of Ca2Al3?pMn3+pSi3O12(OD)-piemontite

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Synthesis experiments of Ca2Al3?pMn3+pSi3O12(OD)-piemontite were performed for the crystal structure analysis and determination of hydrogen positions in epidote structure. The starting materials (S.M.) of oxide mixture with stoichiometric compositions (p = 0.5, 0.75, 1.0 and 1.1) and D2O were used for hydrothermal synthesis experiments at 0.3 GPa and 500 oC. In this study, almost single phase piemontite was synthesized by the run using S.M. with p = 1.0. X-ray data were obtained using conventional X-ray powder diffractometer, and the neutron diffraction data of the piemontite were measured using JRR3-HRPD. The unit-cell parameters given by the X-ray data are a 8.8450(5), b 5.6676(2), c 10.1472(7) A, and beta 115.495(4)o, and the site occupancies at M1 and M3 of Al0.63Mn0.37 and Al0.36Mn0.63, respectively.On the other hand, the unit-cell parameters of a 8.853(1), b 5.6753(4), c 10.159(2) A, and beta 115.49(1)o, and the site occupancies at M1 and M3 of Al0.85Mn0.15 and Al0.15Mn0.85, respectively, were given using a neutron diffraction data. The D position was determined successfully without any constraint.

Keywords: Deutorium, Piemontite, Synthesis, Neutron diffraction, X-ray diffraction, Rietveld analysis