

SMP045-19

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## 含重水素紅簾石の合成と生成相の評価 Synthesis and characterization of D-bearing piemontite

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Ca<sub>2</sub>Al<sub>3-p</sub>Mn<sup>3+</sup>Si<sub>3</sub>O<sub>12</sub>(OH)-piemontites were synthesized at 0.3-0.4 GPa and 500 C using hydrothermal equipment. The run products were analyzed using electron microprobe analyzer and infrared absorption spectral method, and refined using X-ray and neutron powder diffraction methods. The starting materials (s.m.s) of oxide mixture of stoichiometric compositions with p = 0.75, 1.0 and 1.1 and D<sub>2</sub>O were used for hydrothermal synthesis experiments at 0.3-0.4 GPa and 500 deg.C. Starting materials: Oxide mixtures heated at 850 deg.C, and excess D<sub>2</sub>O. Capsule systems: 1) Ag outer capsule with MnO<sub>2</sub>-Mn<sub>2</sub>O<sub>3</sub> buffer + H<sub>2</sub>O; Ag90Pd10 inner capsule with charge + D<sub>2</sub>O; 2) Au outer capsule with MnO<sub>2</sub>-Mn<sub>2</sub>O<sub>3</sub> buffer + D<sub>2</sub>O; Ag90Pd10 inner capsule with charge + D<sub>2</sub>O.

In the present synthesis experiments of deuterium-bearing piemontite using Ag-outer capsule with solid buffer + H<sub>2</sub>O, deuterium was considerably or completely replaced by hydrogen. On the other hand, in the experiments using Au-outer capsule with solid buffer + D<sub>2</sub>O, D-bearing piemontite was synthesized successfully. However, even in this case, seal of Au-outer capsule should be perfect, because hydrogen moves in and out inner Ag90Pd10 capsule.

There is no essential difference for Mn<sup>3+</sup> distributions among octahedral M1, M2 and M3 sites between D-bearing piemontite and H-bearing piemontite: the Mn<sup>3+</sup> occupancies at M1 and M3 in D-bearing piemontite refined using X-ray powder diffraction data are close to those of H-bearing piemontite (Nagashima and Akasaka, 2004). In this study, neutron diffraction data of a D-bearing piemontite synthesized from p = 1.0 starting material at 0.3 GPa and 500 deg.C were measured. Although D in this piemontite was considerably replaced by H because of the use of Ag-outer capsule with solid buffer + H<sub>2</sub>O, D-positions could be refined. Neutron diffraction study of D-bearing piemontite synthesized successfully in this study will give us useful information for the relations between cation substitutions and hydrogen bond.

キーワード: 紅簾石, 熱水合成, 赤外分析, リートベルト解析, 重水素

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