

Cation ordering in Pb²⁺-bearing, Mn³⁺-rich pargasite from Långban, Sweden

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ABSTRACT

A multi-analytical approach using electron microprobe analysis, X-ray structural refinement, and polarized single-crystal Fourier transform infrared spectroscopy was used to characterize short-range and long-range structures of a Pb²⁺-bearing, Mn³⁺-rich pargasite. Site populations, derived from the results of site-scattering refinement and stereochemical analysis, demonstrate that Pb²⁺ is strongly ordered at the A-site in the monoclinic *C2/m* amphibole structure. This finding is in agreement with the observed ordering of Pb²⁺ in the rare Pb²⁺-bearing *P2/a* amphibole joesmithite, but is in contrast to a Pb²⁺ preference for the M4 site suggested by some studies on element partitioning between *C2/m* amphiboles and melts. Mn³⁺ is strongly ordered at the M2 site in structure of the present amphibole. Contrasting results obtained for mean M2-O bond lengths and reported local Mn³⁺-O bond lengths as well as between bond-length distortion of the mean M2 polyhedron and the local Mn³⁺-centered M2O₆ octahedron in pargasite indicates that the structural relaxation of this polyhedron is complete or nearly so.

Keywords: Amphibole, pargasite, lead, manganese, structure refinement, IR spectroscopy