Refinement of Mn-Substituted Muscovite and Phlogopite

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Abstract: The crystal structures of a reddish-purple, Mn-bearing muscovite-2M_1 (alurgite variety) and a reddish-brown, Mn-bearing phlogopite-1*M* (manganophyllite variety) were refined to final residuals of 2.7% and 3.1%, respectively. The refinements were carried out in space groups *C*2/*c* and *C*1 for alurgite and *C*2/*m* and *C*2 for manganophyllite. The *C*1 and *C*2 subgroup refinements gave atomic coordinates consistent with the parent space group refinements. No cation ordering was found in either specimen, and the structures are very similar to those of muscovite and phlogopite. Residual areas of positive electron densities were found between the tetrahedral cations and neighboring oxygens in difference maps of both minerals. Those of alurgite were examined in detail to show the correlation between the residual densities and covalent bonding in the tetrahedra. The valence of the Fe present was determined by Mössbauer spectra as Fe^{3+} in both samples and of the Mn by optical spectra as Mn^{3+} in the alurgite but as Mn^{2+} in the manganophyllite.

Key Words: Alurgite • Crystal structure • Manganese • Manganophyllite • Muscovite • Phlogopite

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