Neutron Diffraction Study of a One-Layer Monoclinic Chlorite

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Abstract: A monoclinic II*b*-2 clinochlore from the Achmatov mine, Ural Mountains, U.S.S.R., was investigated by neutron diffraction. The formula, based on electron microprobe and wet chemical analyses, is $(Mg_{4.54}Al_{0.97}Fe^{2+}_{0.28}Fe^{3+}_{0.18}Mn_{0.01})$ $(Si_{2.85}Al_{1.15})O_{10}(OH)_8$. A refinement based on 512 unique reflections converged in space group C2/m to a final R = .066. Cation disorder was found in the two octahedral positions of the 2:1 layer, whereas partial Mg and Al ordering occurs in the interlayer sheet. The two hydroxyl dipoles are roughly perpendicular to the interlayer sheet, forming weak to medium hydrogen bonds with O...O distances of 2.859 and 2.881 Å. The OH-dipole of the 2:1 layer is perpendicular to the (001) plane.

Key Words: Cation ordering • Chlorite • Crystal structure • Hydrogen bonding • Neutron diffraction

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