Crystal Structure Refinement and Mössbauer Spectroscopy of an Ordered, Triclinic Clinochlore

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Abstract: The crystal structure of a natural, ordered *IIb-4* triclinic clinochlore has been refined in space group $C1^{-}$ from 4282 unique X-ray intensity measurements of which 3833 are greater than 3 times the statistical counting error (3σ). Unit cell parameters are a = 5.3262(6) Å; b = 9.226(1) Å; c = 14.334(3) Å; α = 90.56(2) °; β = 97.47(2) °; and γ = 89.979(9) °, which represents the greatest deviation from monoclinic symmetry yet recorded for a triclinic chlorite. The final weighted R is 0.059 for reflections with $I > 3\sigma$ and 0.064 for all reflections. The chemical formula is $(Mg_{0.966}Fe_{0.034})^{M1}(Mg_{0.962}Fe_{0.038})^{M2}{}_2(Si_{2.96}Al_{1.04})O_{10}(OH)_2(Mg_{0.996}Fe_{0.004})^{M3}{}_2(Al_{0.841}Fe^{III}{}_{0.102}Cr_{0.004}Ti_{0.004})^{M4}(OH)_6$, which is consistent with electron microprobe (EMP), wet chemical analyses, Mössbauer spectroscopy and X-ray structure refinement. The high degree of ordering of the divalent versus trivalent octahedral cations in the interlayer is noteworthy, with Fe^{III} and Al in M4 and virtually no Fe in M3. In the 2:1 layer, M1 and M2 each contain similar amounts of Fe. The 2 tetrahedral sites have nearly identical mean oxygen distances and volumes, and thus show no evidence of long-range cation ordering.

Key Words: Cation Ordering • Chlorite • Clinochlore • Crystal Structure • Mössbauer

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