Refinement of the Crystal Structure of a Monoclinic Ferroan Clinochlore

Audrey C. Rule and S. W. Bailey

Department of Geology & Geophysics, University of Wisconsin Madison, Wisconsin 53706

Abstract: A monoclinic II*b*-2 clinochlore from Washington, D.C., contrary to previous studies, is primarily a ferroan rather than a ferrian chlorite. Disorder of tetrahedral Si,Al cations is indicated because of unsuccessful structural refinements in subgroup symmetries. The true space group is C2/*m*. Slight ordering of Mg, Fe^{2+}, and Fe^{3+} over octahedra M(1) and M(2) within the 2:1 layer (mean M-O,OH = 2.092 and 2.084 Å, respectively), complete ordering of trivalent Al into the centrosymmetric octahedron M(4) of the interlayer sheet (M-OH = 1.929 Å), and ordering of primarily divalent cations (Mg and Fe) into the two interlayer M(3) octahedra (M-OH = 2.117 Å) exist. The excess of negative charge above unity due to tetrahedral substitution of Al for Si (1.378 atoms) is compensated entirely within the octahedral sheet of the 2:1 layer.

Ordering of a trivalent cation into one octahedron in the interlayer should be universal for all stable trioctahedral chlorites. In this specimen the ordering is due to (1) minimization of cation-cation repulsion by layer offsets which provide more space around the trivalent element, and (2) energy minimization by localization of the source of positive charge on the interlayer sheet in one octahedron rather than two. In other structures or for different compositions additional factors can be important also. Most chlorites of the II*b* and *Ib* (β = 90 °) types are expected to show disorder of the tetrahedral cations. The *b* positioning of interlayer and layer provides no preferential driving force for concentration of Si and Al in any tetrahedron as a consequence of the expected ordering of the interlayer cations. The monoclinic II*b*-2 polytype is less abundant in nature than the triclinic II*b*-4 and II*b*-6 structures, because only half as many possible superpositions of layers exist that will produce monoclinic symmetry. Crystallization factors must also be important, because the II*b*-2 chlorite is much less abundant than predicted by this purely geometrical argument.

Key Words: Charge balance • Chlorite • Clinochlore • Crystal structure • Order-disorder

Clays and Clay Minerals; April 1987 v. 35; no. 2; p. 129-138; DOI: 10.1346/CCMN.1987.0350205

Clay Minerals Society (www.clays.org)