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Refinement of the cookeite "*r*" structure

HONG ZHENG* AND STURGES W. BAILEY†

Department of Geology and Geophysics, 1215 West Dayton Street, University of Wisconsin, Madison, Wisconsin 53706, U.S.A.

ABSTRACT

The rare two-layer "*r*" structure of I*aa* cookeite from Little Rock, Arkansas, was refined in space group *Cc* to $R = 7.1\%$. Mean T-O bond lengths of 1.654(1) Å and 1.657(1) Å in one tetrahedral sheet vs. 1.659(1) Å and 1.685(1) Å in the other sheet indicate a partly ordered but asymmetric distribution of tetrahedral Si and Al. The two tetrahedral sheets within the 2:1 layer have different compositions and charges. The Al-rich, higher-charge tetrahedral sheet is thicker and has a closer approach to the interlayer sheet than does the Si-rich, lower-charge sheet. Two Al cations occupy the cis octahedra in the dioctahedral 2:1 layer. Mean M-O,OH bond lengths of 1.946(1), 1.946(1), and 2.110(1) Å in the trioctahedral interlayer sheet indicate a partly ordered distribution of octahedral Al and Li. The Li-rich, lower-charge octahedron in the interlayer is located on a vertical straight line between an Al-rich tetrahedron and a Si-rich tetrahedron. The two higher-charge interlayer Al are located vertically between a Si-rich tetrahedron and the center of a six-membered ring. This pattern of ordering minimizes the cation-cation repulsion inherent in a I*aa* structure and gives the best local charge balance. The protons of the six surface OH groups tilt away from the two Al-rich interlayer sites toward the lower-charge Li site. The details of the interlayer hydrogen bond contacts are influenced by the ordering patterns and the structural distortions present.