Verification of the Triclinic Crystal Structure of Kaolinite

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Abstract: On the basis of neutron diffraction studies, the two inner-hydroxyl ions in highly ordered kaolinite were recently shown to be differently oriented. One of the inner-hydroxyl ions points generally toward a hole in the octahedral sheet and the other toward a hole in the tetrahedral sheet. These orientations and the locations of the other atoms in the primitive triclinic unit cell have now been determined for a sample of Keokuk kaolinite with improved precision compared with that reported earlier. Rietveld structure refinement was carried out for the entire crystal structure simultaneously (99 atom positional and 17 other parameters) with each of two newly collected sets of high-resolution neutron powder diffraction data. The different orientations of the inner-hydroxyl ions are the most marked evidence that the unit cell is not C centered. The positions of the inner-surface hydrogen atoms provide further evidence in that all differ from a C-centered relationship by six to eight estimated standard deviations in their y coordinates. The cell is, therefore, not centered. The space group is *P*1.

Key Words: Inner hydroxyl • Kaolinite • Neutron powder diffraction • Rietveld structure refinement • Tri-clinicity

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