Hydrogen Atom Positions in Kaolinite by Neutron Profile Refinement

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Abstract: A structure refinement of kaolinite made using the Rietveld neutron profile refinement technique has given non-hydrogen atom positions which were not significantly different from those given by B. B. Zvyagin in 1960. All of the hydrogen atoms have been located; the three inner-surface hydrogen atoms are involved in interlayer hydrogen bonds with lengths of 2.95 (4), 2.95(4), and 3.06(4) Å with O-H ... O angles of $168(4)^{\circ}$,and $144(4)^{\circ}$ and $146(4)^{\circ}$ respectively. The inner hydrogen atom is located in a position consistent with that found earlier in dickite and muscovite which are the only dioctahedral layer silicates studied by neutron diffraction to date. The O-H vector makes an angle of 34° with the (001) plane, away from the octahedral sheet, and the projection of the vector on to (001) is at $\sim 30^{\circ}$ to the b axis.

Key Words: Crystal structure • Hydrogen • Kaolinite • Neutron profile refinement • O-H vector • Rietveld method

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