Crystal Structure of Kaolinite: Dimethylsulfoxide Intercalate

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Abstract: The crystal structure of the kaolinite: dimethylsulfoxide (DMSO) intercalate ($P1$, a = 5.187(2), b = 8.964(3), c = 11.838(4) Å, α = 91.53(1) °, β = 108.59(2), γ = 89.92(1) °) has been determined using spectroscopic and X-ray and neutron powder diffraction data. Both the X-ray and neutron powder diffraction patterns were refined. Solid-state ^{13}C, ^{29}Si, and ^{27}Al nuclear magnetic resonance data and previously collected infrared spectroscopic data provided a useful starting model for structural refinement. Due to the extreme overlap of reflections of this low-symmetry unit cell, the Rietveld method proved inadequate, and quasi-single crystal methods were employed. Each DMSO molecule was found to be triply hydrogen bonded above the octahedral vacancy in the gibbsitic sheet of the kaolinite layer. One methyl group is keyed into the ditrigonal hole in the tetrahedral sheet with the other S-C bond parallel to the sheet. The DMSO molecules are accommodated by significant horizontal displacement of individual kaolinite layers to achieve almost perfect overlap of the octahedral vacancy by the adjacent ditrigonal hole.

Key Words: Crystal structure • Dimethylsulfoxide • Infrared spectroscopy • Intercalate • Kaolinite • Neutron powder diffraction • Nuclear magnetic resonance • X-ray powder diffraction

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