Hydroxyl Orientations and Interlayer Bonding in Amesite

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Abstract: The hydroxyl orientations in the $2H_2$ polytype of amesite, $Mg_2Al(SiAl)O_5(OH)_4$, have been determine by minimizing the electrostatic potential energy as a function of OH orientation. The angles, ρ, between the hydroxyls and (001) vary between 81.5 and 88.8 ° . All surface hydroxyls form hydrogen bonds with oxygens of the adjacent layer. The OHs tend to tilt away from the higher charged Al^{VI} ions, and the spread in ρ values is due to variations in the positions of the receptor oxygens. The inner hydroxyls noticeably weaken the interlayer bonding. The substitution of Al in both T and M sites creates a dipolar layer charge and the resulting attraction between layers forms an important part of the interlayer bonding. The $2H_2$ polytype of amesite has substantial interlayer bonding even with all surface hydroxyls replaced by fluorine. This is not true for a composition of $Mg_3Si_2O_5(OH)_4$ where a similar F for OH substitution destroys all interlayer bonding as in kaolinite.

Key Words: Amesite • Fluorine • Hydroxyl orientation • Interlayer bonding • Serpentine

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