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# Comparison of Orientations of OH-Bonds in Layer Silicates by Diffraction Methods and Electrostatic Calculations

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**Abstract:** Orientations of OH-vectors in structural hydroxyl groups of layer silicates were defined both from diffraction data and calculations of electrostatic energy. The comparison of the results showed that for the hydroxyls of the 2:1 layers of chlorites and micas the positions of the hydroxyl protons are mainly determined by electrostatics. For the hydroxyls of dickite, amesite, and the brucitic sheets of chlorite, the results derived by the two methods differed systematically from each other, pointing to a change in the nature of the bond in these OH-groups.

**Key Words:** Chlorite • Dickite • Electrostatic calculations • Hydroxyl vectors • Mica • X-ray diffraction

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