Factors Affecting Orientation of OH-Vectors in Micas

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Abstract: The orientation of the OH-vectors in hydroxyl groups of micas of different compositions, polytype modifications, and symmetry were calculated by the method of minimization of electrostatic energy. The orientations are strongly affected by the peculiarities of structures, and even slight deviations from the ideal dioctahedral periodicity can introduce a correction of as much as 10 ° to the value of the polar angle. Ordering of cations in octahedra lead to twisting of the OH-bond towards the octahedron with lower charge and larger dimension. The latter is less true for cation ordering in tetrahedra. Because of these factors and the dependence of the hydrogen position on the coordinates of heavy atoms, such calculations can give reliable results only if the structure has been refined with high precision. Different polytypes of micas displayed the same orientation of the OH-vectors with respect to the axes of a separate layer, if the stacking sequence did not introduce specific distortions of the 2:1 layer.

Key Words: Celadonite • Electrostatic calculations • Glauconite • Hydroxyl vectors • Mica • Muscovite • Phengite

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