Hydroxyl Orientations in 2:1 Phyllosilicates

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Abstract: The hydroxyl orientations in 31 dioctahedral and trioctahedral 2:1 phyllosilicate structures have been determined by electrostatic energy calculations. These structures included micas, brittle micas, and other related minerals exhibiting ordered as well as disordered cation distributions. The dioctahedral micas and brittle micas were examined with and without the interlayer cation. A range of orientations from 1.3 ° to 183.3 ° (the angle ρ between the O-H and (001) measured with respect to the M1 site) were found. The orientations for the dioctahedral structures represent a continuum of values whereas the trioctahedral species exhibit two possible orientations separated by an energy barrier. One orientation is near 90 ° the other is near 180 °. The latter orientation results from a concentration of charge on the interlayer (IC) and tetrahedral (T) sites at the expense of the octahedral (M) sites. A multiple regression analysis of all 31 structures, using as predictors the *a* and *b* cell parameters, d_{001}, and the charges for T, IC, M1, and M2 sites, was performed. This analysis indicated that the important factors are the charges for IC, T, and M2 sites. When treated as a separate group, one finds the same factors for the dioctahedral structures. The trioctahedral orientations are determined by the charge on the M2 site and the amount of tetrahedral rotation. Using these two predictor equations, the value of ρ can be estimated with a standard deviation of 4.7 ° and 2.9 ° for the dioctahedral and trioctahedral cases, respectively.

Key Words: Brittle Mica • Energy Calculations • Hydroxyl Orientation • Mica • Phyllosilicate

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