
Determination of Illite-Smectite Structures Using Multispecimen X-ray Diffraction Profile Fitting

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Abstract: A procedure for structural investigations by X-ray diffraction of mixed-layer structures incorporating swelling layers has been developed. For each sample, specimens saturated with different cations (Na, Mg, and Ca), are analyzed both as air-dried and as glycolated. One structural model fitting all the observed patterns then provides the structure of the sample. Samples tested include: Illite-smectite (I-S) minerals from Kazakhstan (a rectorite), Dolna Ves in Slovakia, Kinnekulle in Sweden, the North Sea, and Scania in Sweden. The fitting of the patterns of the Kazakhstan rectorite demonstrated that the instrumental parameters applied in the modeling were correct. For the I-S minerals from Slovakia and Kinnekulle the observed patterns were fitted with one two-component I-S model. However, the Ca-saturated and air-dried specimen of the Kinnekulle bentonites had two types of swelling interlayers. For the Slovakian I-S with Reichweite = 2, an alternative two-phase I-S plus I-V (V = vermiculite) model fitted the experimental X-ray diffraction patterns equally well. The I-S mineral from Scania is in fact a three-component I-T-S (T = tobelite) and the North Sea sample is a four-component I-S-V-V', one type of the swelling layers having swelling characteristics intermediately between smectite and vermiculite. In addition to layer types and distribution, interlayer compositions, such as the amount of interlayer glycol and water and of fixed and exchangeable cations, were determined.

Key Words: Illite-Smectite • Simulation • Structure • Swelling • X-Ray Diffraction

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