

**INTERPRETATION OF IR SPECTRA OF MIXED-LAYER ILLITE-SMECTITES  
AND ILLITE-TOBELITE-SMECTITES IN THE REGION OF  
OH-STRETCHING VIBRATIONS**

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Illite-smectite (I-S) and illite-tobelite-smectite (I-T-S) samples of various compositions were studied by infrared (IR) spectroscopy. A special sample preparation technique was used to eliminate the contribution of molecular water. The OH-stretching regions of the spectra were decomposed and curve-fitted, and the individual OH stretching bands were assigned to all the possible types of OH-bonded cation pairs that involve Al, Mg and Fe. The integrated optical densities of the OH bands were assumed to be proportional to the contents of the specific types of OH-linked cation pairs with the absorption coefficients being the same for all individual OH bands. Good agreement between the samples' octahedral cation compositions calculated from the IR data and those given by chemical analysis was obtained for a representative collection of samples in terms of a unique set of individual OH band positions that vary within narrow wavenumber intervals. This has allowed minimizing the ambiguity in spectra decomposition imposed by the poor resolution of smectite spectra and confirmed the validity of the resulting band identification.

For I-S and I-T-S with relatively low proportions of expandable layers (up to 25%) and high total amount of fixed interlayer K and NH<sub>4</sub>, the OH stretching bands attributions found by BESSON & DRITS (1997) for dioctahedral micas was found relevant. For samples having higher proportions of expandable layers, the bands associated with specific OH bonded cation pairs may tend to be shifted to greater wavenumbers with respect to the corresponding bands in micas. In addition to OH bands that refer to the smectite structure, AlOHAl and AlOHFe bands of the pyrophyllite structural fragments were identified.

Unambiguous interpretation of the OH stretching vibrations was found to be possible only for I-S and I-T-S samples with known chemical compositions, so that IR data cannot be used for quantitative determination of octahedral cation composition of mixtures of dioctahedral 2:1 phyllosilicates. In the case of monomineral samples with known chemical compositions, IR data can provide information on the short-range order/disorder in the distribution of octahedral cations along cation-OH-cation directions. This information can be employed, in combination with the data of other spectroscopic and diffraction techniques, in the analysis of two dimensional octahedral cation distribution.

**References**

BESSON, G. & DRITS, V.A. (1997): *Clays Clay Minerals*, **45**: 168-169.