Refined Relationships between Chemical Composition of Dioctahedral Fine-Grained Micaceous Minerals and Their Infrared Spectra within the OH Stretching Region. Part II: The Main Factors Affecting OH Vibrations and Quantitative Analysis

G. Besson[1] and V. A. Drits[2]

[1] CRMD-CNRS-Université, B.P. 6759, 45067 Orleans Cedex 2, France
[2] Geological Institute of the Russian Academy of Sciences, Pyzhevsky Street 7, 109017 Moscow, Russia

Abstract: A new model for the interpretation of dioctahedral mica infrared (IR) spectra in the OH stretching vibration region is proposed. It is based on the analysis of the main factors responsible for the observed sequence of the OH frequencies. In terms of this model, the simple analytical dependence between the OH frequencies and the mass and valency of cations bonded to OH groups has been found. The specific character of the interaction between octahedral Al and OH groups in the mica structures is assumed.

Integrated optical densities of the OH bands determined by the decomposition of the studied mica IR spectra are used for the quantitative analysis, that is, for the determination of a number of each type of octahedral cations per unit cell of the sample under study. A good agreement between the octahedral cation contents of 2:1 layers found from the IR spectra decomposition and the chemical analysis has shown that this technique may be used to study the local order-disorder of isomorphous cation distribution in mica structures.

The essential result obtained by the quantitative analysis of the mica IR spectra is the determination of Fe^{3+} cations in the tetrahedral sites of some samples. This means that the conventional presentation of structural formulae for Al-Fe^{3+}-containing 2:1 layer silicates is unacceptable without consideration of tetrahedral Fe^{3+} by spectroscopic techniques and by the quantitative analysis of the IR spectra, in particular.

Key Words: Cation Mass • Cation Valency • IR Spectra • OH Stretching Frequencies • Quantitative Analysis

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