

**INTERLAYER CATION CHARACTERIZATION IN PHYLLOSILICATES:  
A XANES INVESTIGATION**

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Micas are the most common group of phyllosilicates, minerals that are among the least studied by XAS although being interesting for their two-dimensional structure properties. Micas are structural systems made up of infinite, parallel sheets two-dimensionally extending along the *a* and *b* axes and stacked on *c*\*. The three-dimensional mica structure consists of a composite M module made up of an octahedral sheet sandwiched between two facing tetrahedral T sheets, plus a pseudo-hexagonal planar network of cations, again extending along the *a* and *b* axes, which form the interlayer A. This latter layer is bound to the facing T sheets of two opposite TMT layers by weak ionic forces. Potassium, present in micas only as interlayer cation, is surrounded by two facing distorted hexagonal networks of O atoms belonging to two opposite tetrahedral sheets, with Al, Si and Fe atoms being the tetrahedral centres. In this study we tried to identify and reconstruct, using XANES spectroscopy, the local distortions of the tetrahedral sheets induced by the presence of Fe in both the tetrahedral and octahedral sites, by means of a systematic comparison of powder and single-crystal polarized XANES spectra taken at the potassium *K* edge. Previous XANES investigations performed at the Al, Mg, and Fe *K* edges have already demonstrated correlation between the total Fe content in the octahedral sheet and the overall structural modifications occurring in trioctahedral micas (TOMBOLINI et al., 2002a, b). In this work, using the MXAN code to fit the XANES spectra, we discuss the correlation existing between distortions at the interlayer cation sites and the experimental features at the potassium *K* edge in micas having different Fe concentrations. In these layered structures, the fitting method shows that multiple scattering calculations succeed in measuring the distortions induced by Fe; moreover, the quality of the data greatly depends upon sample orientation with respect to the incident beam direction, so that in-plane and out-of-plane orientations can also be determined. A general reconstruction of the structural environment of the interlayer cations in micas will be presented and discussed.

**References**

- TOMBOLINI, F., BRIGATTI, M.F., MARCELLI, A., CIBIN, G., MOTTANA, A. & GIULI, G. (2002a): Eur. J. Mineral., **14**: 1075-1085.  
TOMBOLINI, F., MARCELLI, A., MOTTANA, A., CIBIN, G., BRIGATTI, M.F. & GIULI, G. (2002b): Int. J. Mod. Phys. B, **16**: 1673-1679.