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Quantification of amorphous and crystalline compounds by QTIR spectroscopy. Example of salitre sediments (Minasgerais, Brazil)

J. BERTAUX, F. FRÖLICH, Ph. ILDEFONSE

ORSTOM, - Labaratoire des Formations Superficielles - UR 12

133

The study of weathering and erosion processes requires to establish a mass balance of minerals from the soils towards the area of sedimentation. This calls for the development of quantitative tools that can be applied for mixtures of very fine and sometimes poorly crystallized minerals found in soils. The results presented here concern the use of FTIR spectroscopy as a quantitative method in such environments.

Samples were prepared using the KBr disc method. This ensures that Beer's law is valid. A quantitave determination of the mineral content from various blends was performed by making a linear decomposition of the mixtures spectrum by the spectra of their constituents. To check the validity of the procedure, the linear decomposition was performed on spectra from artificial mixtures of standard minerals (quartz, kaolinite, gibbsite, calcite, amorphous silica). Good agreements were obtained in the range 1315 - 315 cm-1.

FTIR spectroscopy was used to quantify the mineral constituents of a lacustrine sediment cored at Salitre, Minas Gerais, Brazil. The major phases are organic matter + kaolinite + gibbsite + quartz + amorphous silica (phytoliths and sponge spicules). 53 samples of the core were analyzed. The linear decomposition can be applied for this sediment, provided the IR spectral response of the organic matter is known. "Standard spectra" of organic matter were obtained by analyzing pure organic portion of the sediment, or by subtracting the mineral fraction from the whole spectrum of an organo-mineral sample.

The comparison of quantitative results from FTIR spectroscopy with chemical analyses by ICP-AES demonstrates the pertinence of the method.

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