



The correlation of attenuated total reflectance infrared (ATR-FTIR) spectroscopic data with X-ray diffraction (XRD) parameters and its potential use for mineral identification and quantification in drilling cores: examples from the Pannonian Basin, Hungary

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Four thick sediment sequences in the following boreholes, Vízvár-I (0,0-2965,0 m) in the Dráva Basin, Som-I (999,5-1150,6 m) in southern Transdanubia, and two other boreholes, Doboz-I (3490-4434 m) and Doboz-III (2190-3400 m) in the Békés Basin, Hungary, were investigated in detail. Each drillings cut across Neogene sequences and contain shales, carbonates and clay rocks (Tanács & Viczián, 1995). The selection of these cores is due to the various amounts of smectite, illite and kaolinite minerals that are well manifested during comparison of infrared spectroscopic and former XRD dataset.

During preparation, powdered core samples were settled ($<2\mu\text{m}$ grain size fraction), dried and heated up at 80 °C to minimize the adsorbed water content and then kept in closed vessels covered by parafilm before ATR-FTIR measurements. ATR corrected infrared spectra were converted into numeric parameters corresponding to the band position, height, half-width of band, integrated area and these were, then, correlated with XRD parameters such as height of the reflection, full-width at half maximum (FWHM) of the bands related to different minerals, swelling properties and XRD-based clay mineral content.

In spite of the differences in the data of boreholes, results suggest a good agreement between infrared spectroscopic and XRD parameters for the clay fraction. The quartz, carbonates, kaolinite, mica phases could be identified by both methods in the same proportion in each drillings, and the XRD signal of illite and smectite show the same variability as the spectral features of Si-O and O-H without pre-treatment. The changing illite/smectite ratio also shows good agreement with the increasing degree of vitrinite reflection as an indicator for the maturation of hydrocarbons (Hámor-Vidó & Viczián, 1993).

In the infrared spectra of Som-I cores dickite besides kaolinite and illite was identified, most probably as the alteration product of the lower and middle Triassic limestones. The occurrence of dickite is reported for the first time from similar formation in the Pannonian Basin and it may be an indication of its genesis under deep burial conditions.

References

Tanács, J., Viczián, I. 1995: Mixed-layer illite/smectites and clay sedimentation in the Neogene of the Pannonian Basin, Hungary. - *Geol. Carpath.*, Ser. Clays 4, 1, 3-22.

Hámor-Vidó, M., Viczián, I. 1993: Vitrinite reflectance and smectite content of mixed-layer illite/smectites in Neogene sequences of the Pannonian Basin, Hungary. *Acta Geologica Hungarica*, 36, 197-209.