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Determination of the content and distribution of fixed ammonium in illite-smectite by X-ray diffraction: Application to North Sea illite-smectite

VICTOR A. DRITS,[1] HOLGER LINDGREEN,[2] AND ALFRED L. SALYN[1]

[1]Institute of Geology, Russian Academy of Science, Pyzhevsky per D.7, 109017 Moscow, Russia
[2]Clay Mineralogical Laboratory, Geological Survey of Denmark and Greenland, Thoravej 8, DK 2400 Copenhagen NV, Denmark

ABSTRACT

A new X-ray diffraction method for the determination of the amount and distribution of fixed NH_4^+ in illite-smectite has been developed. Illite-smectite was saturated with K^+ and heated at 150 °C. The 002 and 005 reflections were recorded with steps of 0.01° 2θ, and the experimental *d* values and the values for full-width at half-height (FWHH) were determined using a peak-profile–fitting procedure. Peak profiles were calculated with the NEWMOD program for illite structures having different amounts of NH_4^+ and different patterns for the distribution of NH_4^+ in interlayers. For Upper Jurassic illite-smectite from North Sea oil source rocks, the amount and the distribution of NH_4^+ in illite interlayers were determined by comparing the experimental values for d_{005} and FWHH with the values calculated for the selected illite structures. The amounts of NH_4^+ determined in this manner correlate well with the amounts determined by an isotopic dilution method. The results demonstrate that these illite-smectite samples have K end-member illite and NH_4 end-member illite (tobelite) layers and that the illite layers formed during diagenesis and oil generation actually are tobelite layers.