

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

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### **ABSTRACT**

A new X-ray diffraction method for the determination of the amount and distribution of fixed  $\text{NH}_4^+$  in illite-smectite has been developed. Illite-smectite was saturated with  $\text{K}^+$  and heated at 150 °C. The 002 and 005 reflections were recorded with steps of  $0.01^\circ 2\theta$ , 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  $\text{NH}_4^+$  and different patterns for the distribution of  $\text{NH}_4^+$  in interlayers. For Upper Jurassic illite-smectite from North Sea oil source rocks, the amount and the distribution of  $\text{NH}_4^+$  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  $\text{NH}_4^+$  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  $\text{NH}_4$  end-member illite (tobelite) layers and that the illite layers formed during diagenesis and oil generation actually are tobelite layers.