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Determination of the content and distribution of fixed ammonium in illite-smectite using a modified X-ray diffraction technique: Application to oil source rocks of western Greenland

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ABSTRACT

The X-ray diffraction method previously developed for the determination of the amount and distribution of fixed NH_4^+ in illite-smectite has been modified to include the effects of layer thickness fluctuations of K-saturated and heated smectite and the effects of mean thickness of coherent scattering domains (CSDs). X-ray diffraction patterns and 002 and 005 reflection profiles are calculated for K-saturated and dehydrated NH_4^+-bearing I-S representing models having different distributions of K and NH_4^+ over mica-like interlayers, different proportions of interlayer types, different mean thicknesses of CSDs, and different degrees of thickness fluctuations for K-saturated and heated smectite layers. The diffraction criteria for identification of these models are discussed. The amount of fixed NH_4^+ can be determined accurately from the position of the 005 reflection. Diffraction methods have low sensitivity to different distributions of fixed K and NH_4 over mica-like interlayers in NH_4-bearing I-S containing a high amount of expandable interlayers and a low amount of fixed NH_4. However, the interstratified nature of NH_4-bearing illites or I-S can be determined unambiguously in two limited cases: first, when the structures have a low (<20%) content of expandable layers (W_S) and, secondly, when $NH_4/(NH_4 + K) \geq 0.20$ in the mica-like interlayers, even for $W_S > 0.20$. The method is applied to I-S from western Greenland Cretaceous oil source rocks heated by intrusions. The samples contain I-T-S consisting of 13–33% tobelite layers. Two groups of samples are identified. One includes I-T-S structures in which dehydrated K-smectite layers have no significant thickness fluctuations. For these samples different broadening of 002 and 005 reflections is due only to interstratification of the 9.98 and 10.33 Å layers. In the other group a satisfactory agreement between the experimental and calculated positions and profiles of the 002 and 005 reflections is achieved only when thickness fluctuations for the K-smectite layers are taken into account.