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Semiquantitative determination of trans-vacant and cis-vacant 2:1 layers in illites and illite-smectites by thermal analysis and X-ray diffraction

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ABSTRACT

Interstratified illite-smectites (I/S) and illite-smectite-vermiculites (ISV) representing both hydrothermal and diagenetic transformations and having different degrees of structural order were investigated for cis-trans occupancy in the octahedral sheet by X-ray diffraction (XRD) and by differential thermal analysis (DTA) in combination with evolved water analysis (EWA) using an infrared detector. By XRD, the amounts of cis (w_{cv}) and trans (w_{tv}) vacant 2:1 layers were determined for the three-dimensionally ordered samples using both the WILDFIRE simulation program and calculations based on positions of the 11l and 11$\bar{l}$ reflections. Based on the EWA curves, the I/S and ISV could be divided into three groups having (1) one strong and one or more weak EWA peaks; (2) two well-resolved peaks; and (3) a complex EWA curve. The amounts of cis- and trans-vacant sites were determined by peak fitting of the total dehydroxylation curve. The complex EWA curves were, however, in addition split into separate dehydroxylation processes during a step-heating technique. If the EWA peaks below and above 600 °C were attributed to trans vacant (tv) and cis vacant (cv) octahedra, respectively, the w_{cv} values determined by XRD and by EWA were in agreement. For the three-dimensionally ordered minerals, both XRD and EWA should be used, whereas the EWA method can be applied to the structurally disordered samples having no diagnostic 11l reflections. Accordingly, a combination of XRD and EWA for the determination of w_{cv} and w_{tv} supports an evaluation of the mechanism of illitization in various geological environments. Thus, significant changes in w_{cv} and w_{tv} during illitization are likely due to a dissolution-precipation, whereas almost constant values indicate a solid-state transformation.