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Structural and chemical heterogeneity of illite-smectites from Upper Jurassic mudstones of East Greenland related to volcanic and weathered parent rocks

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ABSTRACT

Illite-smectites (I-S) in one Upper Jurassic mudstone core from East Greenland were investigated to determine their structural and crystal-chemical features and to find the relation between these features and source rocks. The phase composition and layer sequences were determined by X-ray diffraction (XRD), the distribution of octahedral cations over *trans*- and *cis*-octahedra by thermal analysis, the structural formulae by XRD, Mössbauer spectroscopy, and total chemical analysis, and the short-range order in isomorphous cation distribution by infrared (IR) and Mössbauer spectroscopies. For all samples (except one having maximum degree of ordering for R = 1), simulation of the experimental XRD patterns led to two different I-S models having indistinguishable diffraction patterns. For the first, single-phase model, expandability (w_S) is 0.45–0.60. For the second, two-phase model, two randomly interstratified I-S having w_S equal to 0.40 and 0.85, respectively, are present in different proportions in different samples. The single-phase model was selected. A new approach for simulating the two-dimensional distributions of the isomorphous octahedral cations using IR and Mössbauer parameters revealed a tendency for Fe segregation into edge-shared octahedra that may form zigzag chains. Almost identical IR and Mössbauer parameters found for the I-S having different amounts of *trans*-vacant (*tv*) and *cis*-vacant (*cv*) layers (ranging from 0.08 to 0.80) demonstrate that these parameters are largely determined by local cation environments around Fe^{3+} and OH groups. Different levels in the Upper Jurassic Kimmeridgian core contain I-S having different structures. I-S of hemipelagic mudstones at the bottom (37 m depth) and in the middle (13 m depth) of the core, with a high proportion of *cv* layers and of smectite layers (w_S ~ 0.60), probably formed from volcanic material. The other four samples have a high proportion of *tv* layers and probably formed by weathering of micaceous material. One of these I-S, from a mudstone turbidite (at 27 m depth), having maximum degree of ordering for R = 1, probably originated from one type of parent rock, and three mudstones (at depths of 4, 12, and 13 m) with segregated I-S, probably originated from a second rock type.