

Cation redistribution in the octahedral sheet during diagenesis of illite-smectites from Jurassic and Cambrian oil source rock shales

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ABSTRACT

During diagenesis of Jurassic and Cambrian oil source rock shales illite-smectite(-vermiculite) [I-S(-V)] is transformed to illite-tobelite-smectite(-vermiculite) [I-T-S(-V)]. This transformation of S layers to T layers takes place by an increase in tetrahedral charge through Al for Si substitution and subsequent fixation of interlayer NH₄, accompanied by an increase in Al and a decrease in Fe and Mg in the octahedral sheet. In the present investigation, the distribution of isomorphous cations in octahedral sheets of trans-vacant I-S(-V) and I-T-S(-V) was studied by Mössbauer and Infrared (IR) spectroscopies. Mössbauer spectra have been modeled using numerical values of the Fe³⁺ and Fe²⁺ quadrupole doublets corresponding to local cation arrangements around Fe³⁺ and Fe²⁺ in octahedral sheets of micaceous minerals. To interpret IR spectra in the OH-stretching region, frequencies for each pair of cations bonded to OH groups determined for micas and I-S are used. Combination of Mössbauer and IR data by computer simulation provides two-dimensional cation distributions of octahedral cations. The Jurassic and Cambrian I-S(-V) and I-T-S(-V) have clustered octahedral sheets. Ordered clusters of mixed cation composition (Mg, Al, Fe³⁺, and Fe²⁺) with regular alternation of di- and trivalent cations and Fe³⁺-clusters dispersed over an Al-matrix are found in detrital samples. In diagenetically transformed samples, ordered clusters persist while Fe³⁺-clusters degenerate to either short chains consisting of two Fe-Fe pairs or to isolated Fe-Fe pairs oriented along the **b**, **b**₁, and **b**₂ directions. The release of Fe and Mg during diagenesis occurs from Fe³⁺ clusters and through partial destruction of ordered clusters and of **b**₁, **b**₂-oriented Mg-Mg pairs. However, as the cation composition and the short-range cation order within the clusters are preserved and the Al for Fe and Mg substitution occurs at cluster edges, the diagenetic transformation of S (and V) to T layers in both the Jurassic and Cambrian I-S(-V) proceeds through a solid-phase transformation and not through dissolution-reprecipitation.

Keywords: Illite-smectite, cation distribution, computer simulation