

Poster Presentations

[MS18-P02] Structural Investigations of Synthetic Members of Murataite-Pyrochlore Polysomatic Series

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Synthetic analogues of rare mineral murataite, a complex oxide of titanium, iron, rare earth and other elements [1, 2], attract special attention as perspective matrixes for the radioactive waste streams with complex composition. Natural murataite (Mu-3C), space group $F\bar{4}3m$, $a = 14.89 \text{ \AA}$, $Z = 4$, has the ideal and simplified formula $R_6M1_{12}M2_4TX_{43}$ ($R = Y, Na, Ca, Mn$; $M1 = Ti, Fe$; $M2 = Fe, Ti$; $T = Zn$; $X = O, F$) [2]. The crystal structure contains four cation sites: R site is [8]-coordinated, M1 site is octahedrally coordinated, M2 site is [5]-coordinated and T site is tetrahedrally coordinated. The structure is based upon a nanoporous framework consisting of cornerlinked α -Keggin $[Zn^4Ti^6]_{12}O_{40}]^{30-}$ clusters. The framework accommodates complex fluorite-like substructure of Y, Fe and Na cations and O^{2-} and F^- anions.

Transmission electron microscope studies allowed to identify four synthetic murataite varieties with $3 \times 3 \times 3$, $5 \times 5 \times 5$, $7 \times 7 \times 7$ and $8 \times 8 \times 8$ fluorite cubic supercells referred as murataite-3C, -5C, -7C and -8C [3, 4], where murataite-3C corresponds to the natural murataite. Structural investigations reveal that these varieties can be considered as members of murataite-pyrochlore polysomatic series based upon incorporation of high-actinide pyrochlore nanoclusters into modified murataite-like frameworks. Compared to natural murataite, synthetic murataite-3C (cubic, $F\bar{4}3m$, $a = 14.676(15) \text{ \AA}$) has

noticeably less number of vacancies in the cation substructure and contains five instead of four cation positions. Structural and chemical differences between synthetic and natural murataites is the consequence of the significant amounts of fluoride present in natural samples.

The crystal structure of murataite-8C is of outstanding complexity and contains forty symmetrically independent cation positions. It is based upon octahedral framework, which can be described as alternation of murataite and pyrochlore nanoclusters in a three-dimensional chessboard fashion. The nanoclusters are immersed into matrix formed by recombined murataite-pyrochlore matrix with complex structure and composition.

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