Synthesis And Structural Investigation of Novel Barium Molybdenum Hollandite Structures

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Hollandite phases (AxB8O16) exhibit diverse superstructures due to partial occupation and order of the larger "A" cations within the hollandite channels. The relation between the A cations ordering and strongly correlated electron systems, i.e., metal-metal bonded clusters, in hollandite compounds, is not revealed yet. Ba-Mo-hollandite compounds have been previously reported in both triclinic and tetragonal forms. However, experimental data is both scarce and inconsistent, which has greatly contributed to the ambiguity of the cation-ordering mechanism and Mo-Mo bonded clustering within Ba-Mo-hollandite compounds.

In our study, the structure solution of two new incommensurate tetragonal phases, as well as a triclinic phase, was achieved. By using inductively coupled plasma–optical emission spectrometry, the elemental composition of the three phases, was determined. Since the stoichiometry of the three compounds is almost the same, setting clear boundaries between phases in terms of reaction conditions, as well as structural features was done. Structural details were studied using single crystal and powder X-ray diffraction data and later confirmed using the atom probe technique. Furthermore, magnetic measurements were carried out to study the electronic features of Mo clusters. Thus, the interaction mechanism between Mo atoms clustering patterns and the occupancy of Ba atoms is revealed.

Synthesized Ba-Mo hollandites represented a unique case where a link exists between A cations ordering and electron-correlated metal-metal bonded clusters, among hollandite compounds.