

Syntheses, Modulated Crystal Structures of $\text{Ba}_{6-2x}\text{U}_{2+x}\text{Ag}_4\text{Se}_{12}$ ($x = 0$ and 0.5), and Crystal Structure and Spectroscopy of $\text{Sr}_4\text{Th}_{2.78}\text{Cu}_4\text{S}_{12}$

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PII: S0022-4596(18)30354-2
DOI: <https://doi.org/10.1016/j.jssc.2018.08.025>
Reference: YJSSC20343

To appear in: *Journal of Solid State Chemistry*

Received date: 5 June 2018
Revised date: 16 August 2018
Accepted date: 18 August 2018

Cite this article as: Adel Mesbah, Jai Prakash, Jessica C. Beard, Christos D. Malliakas, Sébastien Lebègue and James A. Ibers, Syntheses, Modulated Crystal Structures of $\text{Ba}_{6-2x}\text{U}_{2+x}\text{Ag}_4\text{Se}_{12}$ ($x = 0$ and 0.5), and Crystal Structure and Spectroscopy of $\text{Sr}_4\text{Th}_{2.78}\text{Cu}_4\text{S}_{12}$, *Journal of Solid State Chemistry*, <https://doi.org/10.1016/j.jssc.2018.08.025>

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Syntheses, Modulated Crystal Structures of $\text{Ba}_{6-2x}\text{U}_{2+x}\text{Ag}_4\text{Se}_{12}$ ($x = 0$ and 0.5), and Crystal Structure and Spectroscopy of $\text{Sr}_4\text{Th}_{2.78}\text{Cu}_4\text{S}_{12}$

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ABSTRACT

Single crystals of $\text{Ba}_{6-2x}\text{U}_{2+x}\text{Ag}_4\text{Se}_{12}$ ($x = 0$ and 0.5) and $\text{Sr}_4\text{Th}_{2.78}\text{Cu}_4\text{S}_{12}$ were obtained by standard solid-state chemistry methods at 1173 K. The $\text{Ba}_{6-2x}\text{U}_{2+x}\text{Ag}_4\text{Se}_{12}$ structures are modulated. They were solved and refined in the monoclinic $\text{C2}(\alpha 0 \gamma)0$ super space group. The structure consists of layers formed by the connection of USe_6 and AgSe_4 polyhedra. The incommensurate nature of the structure arises from the disorder among Ba atoms and U atoms in the layers. The crystal structure of the $\text{Sr}_4\text{Th}_{2.78}\text{Cu}_4\text{S}_{12}$ was solved in space group $\text{Pmn}2_1$ of the orthorhombic system. The refinement of the structure reveals three partially occupied Th sites. The connection of ThS_7 and CuS_4 polyhedra form a channel structure filled by Sr atoms. From optical measurements $\text{Sr}_4\text{Th}_{2.78}\text{Cu}_4\text{S}_{12}$ is a semiconductor with an indirect band gap of 2.27(2) eV.

Graphical abstract

View of the substructure of $\text{Ba}_{6-2x}\text{U}_{2+x}\text{Ag}_4\text{Se}_{12}$ nearly down the c axis.

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