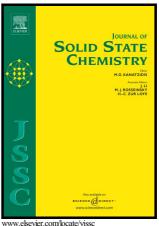
Author's Accepted Manuscript

Syntheses, Modulated Crystal Structures of $Ba_{6-2x}U_{2+x}Ag_4Se_{12}$ (x=0 and 0.5), and Crystal Structure and Spectroscopy of $Sr_4Th_{2.78}Cu_4S_{12}$

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Syntheses, Modulated Crystal Structures of $Ba_{6-2x}U_{2+x}Ag_4Se_{12}$ (x=0 and 0.5), and Crystal Structure and Spectroscopy of $Sr_4Th_{2.78}Cu_4S_{12}$

Adel Mesbah^{a,b}, Jai Prakash^{a,c}, Jessica C. Beard^a, Christos D. Malliakas^a, Sébastien Lebègue^d, James A. Ibers^{a*}

ABSTRACT

Single crystals of $Ba_{6-2x}U_{2+x}Ag_4Se_{12}$ (x = 0 and 0.5) and $Sr_4Th_{2.78}Cu_4S_{12}$ were obtained by standard solid-state chemistry methods at 1173 K. The $Ba_{6-2x}U_{2+x}Ag_4Se_{12}$ structures are modulated. They were solved and refined in the monoclinic $C2(\alpha0\gamma)0$ 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 $Sr_4Th_{2.78}Cu_4S_{12}$ was solved in space group $Pmn2_1$ 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 $Sr_4Th_{2.78}Cu_4S_{12}$ is a semiconductor with an indirect band gap of 2.27(2) eV.

Graphical abstract

View of the substructure of $Ba_{6-2x}U_{2+x}Ag_4Se_{12}$ nearly down the c axis.

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^aDepartment of Chemistry, Northwestern University, 2145 Sheridan Road, Evanston, IL 60208-3113, United States. ^bICSM, UMR 5257, CEA CNRS, ENSCM, Univ. Montpellier, Site de Marcoule-Bât.426, BP 17171, 30207 Bagnols-sur-Cèze, France.

^cDepartment of Chemistry, Indian Institute of Technology Hyderabad, Kandi 502 285, Sangareddy, Telangana, India. ^dLaboratoire de Physique et Chimie Théoriques (LPCT, UMR CNRS 7019), Institut Jean Barriol, Université de Lorraine, BP 239, Boulevard des Aiguillettes, 54506 Vandoeuvre-lès-Nancy (France)

^{*}Corresponding author: E-mail address: ibers@chem.northwestern.edu (J.A. Ibers)

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