Exploratory syntheses and crystal chemistry of new complex multinary chalcogenides

Jai Prakash

Department of Chemistry, Indian Institute of Technology Hyderabad, Sangareddy, Medak District, India

Email: jaiprakash@chy.iith.ac.in

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The structural aspects of metal chalcogenides have been actively studied for a long time, mainly by solid-state chemists and mineralogists, owing to their rich crystal chemistry. In the last few decades, the study of structure-property relationships of these chalcogenides has become one of the thrust areas of research in the field of materials sciences. These chalcogenides are important for diverse technological applications such as thermoelectric materials, data storage, photovoltaics, magnetism, charge and spin density wave, superconductivity, etc. In recent years, complex metal chalcogenides, especially tellurides, have been explored for their promising thermoelectric properties. We have been actively working on the exploratory syntheses and characterization of new semiconducting mixed metal ternary and quaternary chalcogenides. Our efforts have led to the discovery of various multinary chalcogenides with unprecedented structure types in the last few years. The single crystals X-ray diffraction studies determined these phases' crystal structures at room temperature. The crystal structures of these compounds are anisotropic in nature (Fig. 1). The structural aspects of these new compounds, namely $A_kScMQ_3$ ($A_k = Sr$ and $Ba$; $Q = S, Se$, and $Te$) [1], $Ba_{2-\delta}Ln_{1-x}Mn_2Q_5$ ($Ln =$ lanthanides) [2], $Ba_4Ge_2Sb_2Te_{10}$ [3], and $Ba_4FeAgS_6$ [4] will be presented in detail along with their relationship with other known structures of metal chalcogenides. The transition metals (or main group metalloids), lanthanides, and chalcogen atoms in these structures form anionic frameworks. The alkaline-earth metal cations mainly act as electron donors and are stuffed in the open spaces of these anionic frameworks. Optical absorption and temperature-dependent resistivity studies show that these compounds are narrow bandgap semiconductors, which could be promising for future thermoelectric (TE) applications. Understanding the structural relationship among these structure types is vital for discovering and designing new compounds with desired physical properties.

![Figure 1](image)

**Figure 1.** The unit cell structures of (a) $BaLnCuQ_3$, (b) $BaScAgTe_3$, (c) $Ba_2Ln_{1-x}Mn_2Te_5$, and (d) $Ba_4FeAgS_6$.


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