

New quaternary $I_4-II-IV_2-VI_7$ chalcogenides with diamond-like structures.

Stanislav S. Stoyko, Joshua Kotchey, Evan O'Hara and Jennifer A. Aitken
Duquesne University

Over the past decade multinary chalcogenides, especially those with the diamond-like structures, have been attracting considerable attention due to their promising, tunable thermoelectric, photovoltaic and non-linear optical properties. The formulae of quaternary compounds with diamond-like structures, for example $I_2-II-IV-VI_4$, can be predicted through the employment of valence electron and Pauling's rules. These compounds are non-centrosymmetric with all cations adopting tetrahedral environment and with all tetrahedra pointing in a single direction. A series of new quaternary $I_4-II-IV_2-VI_7$ chalcogenides with two different diamond-like structures, crystallizing in space groups $C2$ and Cc , were successfully accessed through the employment of the described rules in combination with isovalent substitutions of elements and with the tuning of arrangement of tetrahedral units. This presentation will describe crystal and electronic structures of new $I_4-II-IV_2-VI_7$ chalcogenides, as well as their relationship with other, known-to-date diamond-like structures and their potential for technological applications.