

Inverse Clathrates: Formation, Crystal Chemistry and Thermoelectric Properties

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Besides the general class of intermetallic clathrates bearing positively charged fillers like Cs, Sr or Ba inside the cages, there also exist the so-called inverse clathrates incorporating group VI (Te) or VII (Cl, Br, I) elements. Up to now approximately 40 different compounds were reported for this class. This work provides a comprehensive compilation of investigations performed hitherto on these compounds [1]. Despite most of the compounds reported crystallize in the clathrate type-I structure, a wide range of different superstructures is observed for inverse clathrates due to atom or vacancy ordering. Similar to the polyanionic clathrates features like the rattling of the guest atoms were reported for inverse clathrates, and thus they are considered as potential thermoelectric materials. Most of the compounds exhibit semiconducting behaviour with a p-type electrical conductivity. Although substitution allows modifying the thermoelectric properties, for most of them the high electrical resistivity does not allow to achieve attractive ZT-values.

[1] M. Falmbigl, P. Rogl, *Thermoelectric Inverse Clathrates*, submitted.