

X-ray Diffraction Studies of two Germanium $\text{Sr}_8\text{Ga}_{16}\text{Ge}_{30}$ and $\text{Cs}_8\text{Na}_{16}\text{Ge}_{136}$ Clathrates: Promising Candidates for Thermoelectric Applications

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X-ray diffraction patterns of Type I (semiconducting $\text{Sr}_8\text{Ga}_{16}\text{Ge}_{30}$) and Type II (metallic $\text{Cs}_8\text{Na}_{16}\text{Ge}_{136}$) clathrate compounds have been prepared using the X-ray Rietveld refinement technique. These compounds feature zeolite-like open structures, and have potential thermoelectric applications. The type I $\text{Sr}_8\text{Ga}_{16}\text{Ge}_{30}$ compound crystallizes in $Pm-3n$ with $a = 10.73377(8) \text{ \AA}$, and the type II $\text{Cs}_8\text{Na}_{16}\text{Ge}_{136}$ phase is also cubic with space group $Fd-3m$ and $a = 15.48463(38) \text{ \AA}$. The frameworks of these compounds are characterized by covalent tetrahedrally-bonded (Ge,Ga) or Ge atoms, which form polyhedral cages inside which the alkali/alkaline-earth metals are located. While the sizes of the two cavity types in the Type I structure are similar, they are significantly different in the Type II structure. X-ray powder diffraction patterns of these two compounds have been submitted to ICDD to be included in the Powder Diffraction File. The structure of $\text{Na}_{1-x}\text{Ge}_3$ which often coexists with the type-II clathrate $\text{Na}_x\text{Ge}_{136}$ phase during the synthesis process will also be discussed.