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Direct verification of Ga-Ga bond avoidance in the clathrate $Ba_8Ga_{16}Sn_{30}$ from EXAFS studies MICHAEL KOZINA, F. BRIDGES, Y. JIANG, UC Santa Cruz, M. AVILA, Universidade Federal do ABC, K. SUEKUNI, T. TAKABATAKE, Hiroshima University — $Ba_8Ga_{16}Ge_{30}$ and $Ba_8Ga_{16}Sn_{30}$ are important thermoelectric clathrate materials with low thermal conductivities. In these materials, the Ga/Ge or Ga/Sn atoms occupy three sites in the cage-like lattice, but the Ga are not randomly distributed. Experiments in the past have only been able to suggest that Ga-Ga bonds are not favored within the cage structure of many type I clathrates. Here we show definitive evidence that this is indeed the case for $Ba_8Ga_{16}Sn_{30}$. Using the EXAFS technique, we are able compare the backscattering functions for the first neighbors about Ga to the calculated functions for Ga-Ga and Ga-Sn bonds. The result is that only $\sim$15% of the Ga nearest neighbors are Ga. Combining this result with diffraction data on occupational parameters, we propose one possible arrangement of Ga and Sn in the unit cell of $Ba_8Ga_{16}Sn_{30}$. Additionally, we find significant disorder in the Ga/Sn lattice; the Ga-Sn bond and Ga-Ga bonds are 0.07Å and 0.2Å (respectively) shorter than the average bond length, which must contribute to the smaller thermal conductivity.

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