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Large local distortions around the Ba site in $Ba_8Ga_{16}X_{30}$, X=Si, Sn[1] TREVOR KEIBER, Univ of California-Santa Cruz, FRANK BRIDGES, PATRICK NAST, UC Santa Cruz, SCOTT MEDLING, Australian National University, TOSHIRO TAKABATAKE, Hiroshima University — We report an Extended X-ray Absorption Fine Structure (EXAFS) analysis of thermoelectric type-I clathrates, $Ba_8Ga_{16}X_{30}$, X=Sn,Si. These clathrates have a cage-like crystal structure filled with "rattler" atoms (Ba) located near the center of the cages (Ga-X). In contrast to the results for $Ba_8Ga_{16}Ge_{30}$, our results show that for X=Sn,Si the average pair distances within the cages (Ga-Sn, Ga-Ga, Ga-Si, Sn-Sn) are significantly different than the average distances found from diffraction. Direct measurements of the Ba K edge suggests that the environment about Ba is very highly disordered for X=Sn,Si compared to X=Ge, with surprisingly short Ba-X/Ga distances; likely the Ba2 site is significantly off center. For Si, the Ba K first neighbor peak is substantially reduced in size and shifted to lower r due to interference effects from many different Ba neighbor distances. For X=Sn the Ba-Ga/Sn distances are even shorter, and there is a split peak with very low amplitude suggesting a very disordered environment. The mixed distances of the cage atoms, the very short Ba-Ga/X distances, as well as the disorder about the Ba site, suggest that the cage structure is buckled. This disorder will lead to increased scattering for both phonons and electrons.

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