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NMR and computational modeling of $Ba_8Ga_{16}Sn_{30}$ clathrates SERGIO Y. RODRIGUEZ, XIANG ZHENG, JOSEPH H. ROSS, JR., Department of Physics and Astronomy, Texas A&M University, College Station TX 77843 — We report studies of $Ba_8Ga_{16}Sn_{30}$ clathrates by NMR and modeling in order to better understand the electronic and dynamical properties. For samples exhibiting both the type-I and type-VIII clathrate structures, we have measured ^{71}Ga quadrupole NMR lineshapes. We used *ab initio* modeling to extract structural information, providing an estimate of the site-occupation preferences in these alloys. For the type-I material, the resulting preferred structures are similar to those obtained in type-I $Ba_8Al_{16}Ge_{30}$, and we also find that the calculated formation energies show a preference for local structures that are similar to those of the BaAlGe analog. NMR Knight shifts at high temperatures are constant indicating metallic behavior. *Ab initio* results are in partial agreement with the local distribution of this metallic behavior. However the NMR lineshapes and T_1 relaxation time show low temperature changes in type-I samples attributed to atomic dynamics, which we connect to the prominent rattling behavior in this clathrate. Supported by Robert A. Welch Foundation (Grant A-1526).

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