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**NMR and computational modeling of  $\text{Ba}_8\text{Ga}_{16}\text{Sn}_{30}$  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  $\text{Ba}_8\text{Ga}_{16}\text{Sn}_{30}$  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  $^{71}\text{Ga}$  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  $\text{Ba}_8\text{Al}_{16}\text{Ge}_{30}$ , and we also find that the calculated formation energies show a preference for local structures that are similar to those of the  $\text{BaAlGe}$  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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