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NMR relaxation and phonon rattling in type-I $Ba_8Ga_{16}Sn_{30}$ clathrates XIANG ZHENG, SERGIO Y. RODRIGUEZ, JOSEPH H. ROSS, JR., Department of Physics and Astronomy, Materials and Engineering Program, Texas A&M University — The atomic motion of guest atoms inside clathrate cages has been considered as one of the important reasons for the observed glasslike thermal behavior. ^{69}Ga and ^{71}Ga Nuclear Magnetic Resonance (NMR) studies of type-I $Ba_8Ga_{16}Sn_{30}$ clathrates show a clear low temperature spin-lattice relaxation peak attributed to the influence of Ba rattling dynamics on the framework-atom resonance. Analysis indicates that the quadrupolar relaxation is the leading contribution. The data are analyzed using a two-phonon Raman process, according to a recent theory involving localized one dimensional anharmonic oscillators. Excellent agreement is obtained using this model, with the parameters corresponding to a double well with very large anharmonicity. We have extended the theory to include a two dimensional anharmonic well, with similar parameters providing the best fit to the data. We also examine the Einstein type peak observed in heat capacity using this model, and compare to previous reported results obtained using different models for the anharmonic oscillator. This work is supported by Robert A. Welch Foundation (A-1526).

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