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$Ba_8Ga_{16}Sn_{30}$ type-I clathrate NMR lineshape simulations SERGIO Y. RODRIGUEZ, XIANG ZHENG, LAZIZ SARIBAEV, JOSEPH H. ROSS, JR., Texas A&M University — Semiconductor clathrates consist of Si, Ge or Sn networks containing guest atoms. Clathrates have gained considerable attention due to their potential for thermoelectric device application. To understand the Ga substitutional configuration and Ga-Ga bonding, we calculated Ga NMR lineshapes for type-I $Ba_8Ga_{16}Sn_{30}$. The results were obtained by calculating Electric Field Gradients (EFG) for different Ga framework occupation. To obtain the EFG's we used *ab initio* methods with the Generalized Gradient Approximation for the exchange-correlation term as implemented in the WIEN2k code. These were compared with our experimental NMR lineshapes. By x-ray-absorption fine structure technique simulations it had previously being suggested that the number of Ga-Ga bonds was between 4 and 5. Our results showed that this number should be lower due to the mismatch between the experimental and simulated NMR lineshapes. Furthermore it was obtained that Ga-Ga bonds on $16i$ adjacent sites are not energetically favorable. EFG's corresponding to such configurations are also extremely large and do not agree with our measured NMR lineshapes. On the other hand we found good agreement between the measured lineshapes and the configuration with the lowest computed energy. This work was supported by Robert A. Welch Foundation (Grant A-1526).

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