Calculation of NMR lineshapes for Ba-Al-Ge clathrates SERGIO RODRIGUEZ, WEIPING GOU, JOSEPH ROSS, Texas A&M University — Clathrates consist of Si, Ge, or Sn cages in a crystalline framework, with guest atoms inside the cages. They have gained interest due to thermoelectric properties suitable for potential device application. To understand Al substitutional configurations, we calculated Al NMR line shapes for several structures with compositions $Ba_8Ge_{46-x-y}Al_x\square_y$ for $x = 3, 8, 11, 12, 16, 24$; $y = 2, 3$; where $\square$ represents a vacancy. The results were obtained by calculating Electric Field Gradients (EFG) for Al sites of type-I clathrates assuming an ordered superstructure of vacancies and framework occupation. We used *ab initio* methods in the Generalized Gradient Approximation as implemented by the WIEN2k program, and used the results to simulate NMR lineshapes numerically. These were compared to our previously reported NMR lineshapes. In the case of $Ba_8Ge_{31}Al_{12}\square_3$ four Al sites in the superstructure include two sites with small EFG where the vacancy is far away and two sites with large EFG with a vacancy adjacent to Al. Assuming a larger Knight shift for sites next to vacancies, we obtain good agreement with NMR experimental results for reduced-Al $Ba_8Ge_{34}Al_{12}$, while for the Zintl phase $Ba_8Ge_{30}Al_{16}$ we obtain good agreement with no spontaneous vacancies. We infer that Al prefers locations close to vacancies rather than random occupation. This work was supported by Robert A. Welch Foundation (Grant A-1526).

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