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NMR Studies of Ba8AlxGe46-x and Ba8GaxGe46-x Clathrates
GOU WEIPING, YANG LI, JI CHI, V. GORUGANTI, K. D. D. RATHNAYAKA, JOSEPH H. ROSS, JR., Department of Physics, Texas A&M University — We have prepared a series of clathrates of the general form, $Ba_8Al_xGe_{46-x}$. X-ray measurements indicate that Al occupies predominantly the $24k$ site, similar to previous observations for the Ga analogs. ^{27} NMR measurements using wide-line and MAS spectrometers indicate two different local Al sites, one with a relatively small quadrupole splitting, attributed to the $24k$ site, and one with a larger quadrupole splitting attributed to Al adjacent to a vacancy. We also discuss the results of *ab-initio* calculations supporting these conclusions. T-dependent NMR relaxation results show roughly Korringa-type behavior for both series of compounds for $x < 16$, characteristic of heavily-doped semiconducting materials. The lowest-carrier density Ga_{16} sample shows changes in T_1 and Knight shift characteristic of incipient localization at low temperatures, however analysis indicates that the carriers remain in the regular band rather than forming an impurity band. For Ga_x clathrates synthesized from excess Ga, the NMR T_1 changes abruptly, indicative of a change in band-edge symmetry for p-type material. This work was supported by the Robert A. Welch Foundation (grant A-1526), and the National Science Foundation (DMR-0103455).

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