

Abstract Submitted
for the TSF07 Meeting of
The American Physical Society

Experimental study of $\text{Ba}_8\text{Al}_x\text{Ge}_{46-x}$ clathrates by NMR and other techniques¹ WEIPING GOU, JI CHI, YANG LI, V. GORUGANTI, JOSEPH H. ROSS, JR., Department of Physics, Texas A&M University — Cage-structured group-IV clathrates exhibit interesting properties, for example very high thermoelectric efficiency. We have investigated $\text{Ba}_8\text{Al}_x\text{Ge}_{46-x}$, which is a ternary semiconductor for the case $x = 16$. ^{27}Al NMR studies for $x = 16$ show metallic behavior, indicating doping by native defects into the metallic regime. For smaller x the average relaxation rate increases, indicating an increased density of carriers. We also observe vacancies in low- x samples via electron microprobe studies. For $x = 12$ and 13, NMR exhibits a second line not seen for $x = 16$, attributed to Al adjacent to vacancies. Magic angle spinning NMR and computer simulation of the first-order quadrupole line shape for these samples were used to analyze the observed NMR lines. In addition, we have used ab initio calculations of the electric field gradients to match the observed quadrupole broadening with the local structure. Evidence indicates that Al adjacent to vacancies are predominantly on $24k$ sites. These sites have significantly different local electronic structure and smaller density of conduction electrons.

¹This work was supported by the Robert A. Welch Foundation (grant A-1526), and the National Science Foundation. *Y. Li Present address: Dept. Engineering Sciences and Materials, U. Puerto Rico at Mayaguez

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Date submitted: 05 Oct 2007

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