

Abstract Submitted
for the NWS19 Meeting of
The American Physical Society

Formation enthalpy of a four-defect in GdAl_2 ¹ WINDY OLSEN, GARY S COLLINS, Physics and Astronomy, Washington State University — GdAl_2 has the cubic Laves crystal structure. Indium solute atoms were previously observed to occupy both Gd- and Al-sites with site-fractions that varied in response to changes in composition or temperature [1]. Five Al-rich samples exhibited a transfer enthalpy for In of 0.343(7) eV between the two sublattices [1]. It was assumed in that study that the deviation from stoichiometry was sufficiently great that all point defects were structural and their mole fractions were independent of temperature. New analyses for other samples having compositions much closer to stoichiometry appear to show an equilibrium transfer enthalpy that is much smaller, close to 0.00 eV. The difference in enthalpies was shown in [1] to equal one-fourth of the activation enthalpy to form a thermally-activated combination of four elementary defects: 3 Al-vacancies and one Al-antisite atom on the Gd-sublattice. One can therefore infer a formation enthalpy of $4 \times 0.34 \text{ eV} = 1.36 \text{ eV}$ for the four-defect combination. [1] Matthew O. Zacate and Gary S. Collins, Phys. Rev. B69, 174202 (2004).

¹Supported in part by the National Science Foundation under grant DMR 18-09531.

Gary Collins
Physics and Astronomy, Washington State University

Date submitted: 11 Apr 2019

Electronic form version 1.4