

Abstract Submitted  
for the MAR11 Meeting of  
The American Physical Society

**Einstein Modes in the Phonon Density of States of the Single-Filled Skutterudite  $\text{Yb}_{0.2}\text{Co}_4\text{Sb}_{12}$**  IVO K. DIMITROV, Brookhaven National Laboratory, MICHAEL E. MANLEY, Lawrence Livermore National Laboratory, STEVEN M. SHAPIRO, Brookhaven National Laboratory, JIONG YANG, WEN-QING ZHANG, LIDONG CHEN, Shanghai Institute of Ceramics, Chinese Academy of Sciences, QING JIE, Brookhaven National Laboratory, GEORG EHLERS, ANDREY PODLESNYAK, Spallation Neutron Source, Oak Ridge National Laboratory, JORGE CAMACHO, QIANG LI, Brookhaven National Laboratory — Measurements of the phonon density of states by inelastic neutron scattering and specific heat measurements along with first principles calculations, provide compelling evidence for the existence of an Einstein oscillator (*rattler*) at  $\omega_{E1} \approx 5.0$  meV in the filled skutterudite  $\text{Yb}_{0.2}\text{Co}_4\text{Sb}_{12}$ . Multiple dispersionless modes in the measured density of states of  $\text{Yb}_{0.2}\text{Co}_4\text{Sb}_{12}$  at intermediate transfer energies ( $14 \text{ meV} \leq \omega \leq 20 \text{ meV}$ ) are exhibited in both the experimental and theoretical *density of states* of the Yb-filled specimen. A peak at 12.4 meV is shown to coincide with a second Einstein mode at  $\omega_{E2} \approx 12.8$  meV obtained from heat-capacity data. The emergence of local modes at intermediate transfer energies is attributed to altered properties of the host  $\text{CoSb}_3$  cage as a result of Yb filling. It is suggested that these modes are owed to a complementary mechanism for the scattering of heat-carrying phonons in addition to the mode observed at  $\omega_{E1} \approx 5.0$  meV.

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Date submitted: 16 Nov 2010

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