

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Vibrational dynamics of AV_2Al_{20} ($A = \text{Sc, La and Ce}$) cage compounds ANDREAS LEITHE-JASPER, MPI-CPfS, MAREK KOZA, ILL, Grenoble, YURI GRIN, MPI-CPfS — We report on the inelastic response of AV_2Al_{20} (with $A = \text{Sc, La and Ce}$) probed by high-resolution inelastic neutron scattering experiments [1]. Intense signals associated with the dynamics of Sc, La and Ce are identified in the low-energy range at 6-14 meV in ScV_2Al_{20} and at 8-16 meV in LaV_2Al_{20} and CeV_2Al_{20} . Their response to temperature changes between 2 and 300 K reveals a very weak softening of the modes upon heating in LaV_2Al_{20} and CeV_2Al_{20} and a distinguished blue shift by about 2 meV in ScV_2Al_{20} . By means of density functional theory (DFT) and LDC we show that the unusual anharmonicity of the Sc-dominated modes is due to the local potential of Sc featured by a strong quartic term and compare it with anharmonic systems $(Al,Ga)V_2Al_{20}$ [2]. [1] M. M. Koza et al., Phys. Chem. Chem. Phys. **16**, 27119 (2014) [2] M. M. Koza et al., Phys. Chem. Chem. Phys. **17**, 24837 (2015)

Andreas Leithe-Jasper
MPI-CPfS

Date submitted: 07 Nov 2016

Electronic form version 1.4