

Abstract Submitted
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Rattler

behavior in As skutterudites and oxy-skutterudites¹ FRANK BRIDGES, BRAD CAR, MIKAELA HOFFMAN-STAPLETON, TREVOR KEIBER, LOGAN SUTTON, UC Santa Cruz, M. BRIAN MAPLE, UC San Diego — We report EXAFS measurements for the series $\text{CeX}_4\text{As}_{12}$ ($X = \text{Fe, Ru, Os}$) and $\text{NdCu}_3\text{Ru}_4\text{O}_{12}$ as a function of temperature for most elements in the structure. In each case the rare earth atom is a “rattler” atom, with a low Einstein temperature while the skutterudite cage structure is relatively stiff. From temperature dependencies of the correlated Debye model for the cage atoms, one can estimate the effective spring constant for various atom pairs. We also find for the oxy-skutterudites that the planar CuO_4 sub-structure is very stiff, and likely vibrates as a rigid unit. We compare the behavior of the As-skutterudites with other skutterudites and with the oxy-skutterudites, and discuss in terms of the rigid cage model. The second neighbor pair Ce-X for the As-skutterudites is softer than expected while for the oxy-skutterudites the second neighbor Nd-Ru pair is stiffer than the nearest neighbor Nd-O pair. Models are need to explore this behavior.

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