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Physical properties from $Na_{24}Si_{136}$ single crystals[1] M. BEEKMAN, Department of Physics, University of South Florida, W. SCHNELLE, M. BAITINGER, H. BORRMANN, K. MEIER, Max-Planck-Institut fur Chemische Physik fester Stoffe, A. DATTA, Department of Physics, University of South Florida, YU. GRIN, Max-Planck-Institut fur Chemische Physik fester Stoffe, G.S. NOLAS, Department of Physics, University of South Florida — The first investigation of intrinsic physical properties from single crystals of a Na_xSi_{136} ($0 \leq x \leq 24$) member is reported. Clathrate-II $Na_{24}Si_{136}$ specimens were prepared by a novel method employing spark plasma treatment of the precursor Na_4Si_4. The magnitude and temperature dependence of the electrical and thermal transport is understood in the context of metallic conduction, while magnetic susceptibility data indicate sharp features in the electronic density of states near the Fermi level. An Einstein-like vibrational mode that can be attributed to Na guest "rattling" is clearly observed through a pronounced contribution to the heat capacity, and explains the exceptionally large atomic displacement parameter for Na obtained from single crystal X-ray diffraction data. The experimental data are in very good agreement with prior electronic structure calculations.

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