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Tunneling and Rattling in the Intermetallic Cage Compound $VAl_{10+\delta}$ DOUGLAS SAFARIK, TOMASZ KLIMCZUK, DARRIN BYLER, JASON LASHLEY, Los Alamos National Laboratory — We have used a variety of thermodynamic and transport measurements to study the low-energy "rattling mode" in the so-called "Einstein solid," $VAl_{10+\delta}$ [1]. The rattling is thought to arise from weakly bound Al atoms that occupy the large void at the center of Z_{16} Friaf polyhedra, of which there are eight per unit cell in the $VAl_{10+\delta}$ structure. We find that the temperature dependence of our heat capacity and electrical resistivity data are indeed consistent with an Einstein oscillator-type localized mode. In contrast, we find that the T-dependence of our elastic constant and internal friction data deviate significantly from that expected for an Einstein oscillator. Indeed, the moduli data show a local minimum at $\sim$20 K, followed by a broad local maximum centered at $\sim$40 K, whereas in the same temperature range the internal friction data show a peak. Both of these observations strongly suggest that the atom inside the polyhedron undergoes quantum mechanical tunneling. We propose a model for the interatomic potential inside the polyhedron that accounts for both the rattling and tunneling behavior.

[1] A. D. Caplin, G. Grüner, and J. B. Dunlop, Phys. Rev. Lett. **30**, 1138 (1973).

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