

Abstract Submitted
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Phase transitions and ferroelectricity in $\text{NaSb}_3\text{F}_{10}$ PETER WU, PANOS PHOTINOS, SIDNEY ABRAHAM, JASON MATTHEWS¹, R. CHRISTIE, Southern Oregon University — The structural prediction that $\text{NaSb}_3\text{F}_{10}$ is a new ferroelectric has been confirmed experimentally. The mean phase transition temperature $T_C \approx 461$ K with an associated entropy change ~ 6 J mol⁻¹ K⁻¹. The colorless crystals melt at $T_m \sim 515$ K with decomposition starting at ~ 600 K. A thermal hysteresis in T_C of ~ 35 K between heating and cooling at 25 K min⁻¹ is typical of a first order phase transition. The space group in ferroelectric phase III is $P6_3$, that in the predicted antiferroelectric phase II is $P6_322$, a supergroup of $P6_3$. The space group of prototypic nonferroic phase I is supergroup $P6_3/mmc$, of which the space group of phase III is not a subgroup. The dielectric permittivity at 100 Hz increases more than an order of magnitude from 350 K before undergoing a major inflection at $T_C = 460(10)$ K; it increases thereafter to T_m . The dielectric loss at 100 Hz is low but increases an order of magnitude from its value at ~ 350 K before undergoing an inflection at ~ 460 K, also rising steadily thereafter to T_m . The reproducible dielectric hysteresis loop, with $P_S \approx 20\mu$ C m⁻² at room temperature under the application of 0.3 MV m⁻¹ a.c. or greater, unambiguously verifies the predicted ferroelectric property. The pyroelectric coefficient $\langle p \rangle = 17(5)\mu$ C m⁻² K⁻¹ at 298 K.

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