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Synthesis and characterization of the charge-transfer insulator \mathbf{KCuF}_3^1 SHI YUAN, Dept. of Physics and Materials Research Laboratory, University of Illinois at UC, J.C.T. LEE, P. ABBAMONTE, S.L. COOPER — KCuF₃ is thought to be a prototypical orbital ordering material, with interesting properties that include a highly anistotropic superexchange ratio and one-dimensional spin dynamics down to a very low energy and temperature scale. High-quality single crystals of KCuF₃—with a typical size of roughly $3.6 \times 3.6 \times 2.5$ mm³—were grown using an aqueous solution precipitation method. Room temperature x-ray powder diffraction measurements using Cu K_{α} radiation showed that the samples consisted of >90% volume fractions of polytype a. Temperature-dependent Raman measurements provide evidence for structural instabilities between 50K and 300K in $KCuF_3$, including a decrease with decreasing temperatures ("softening") of several phonon mode frequencies, and phonon mode splitting near 50K consistent with a tetragonalto-orthorhombic (TO) transition that precedes the Néel transition at 40K. We argue that the TO structural transition is associated with rigid GdFeO₃-type rotations of the CuF_6 octahedra.

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