Unusual structural evolution in KCuF$_3$ at high temperatures by neutron powder diffraction$^1$ LUKE G. MARSHALL, JIANSHI ZHOU, Materials Science and Engineering Program, University of Texas at Austin, JIANZHONG ZHANG, JIANTAO HAN, SVEN C. VOGEL, XIAOHUI YU, LANSECE Division, Los Alamos National Laboratory, YUSHENG ZHAO, LANSECE Division, Los Alamos National Laboratory; Department of Physics and Astronomy, University of Nevada, MARIA-TERESA FERNANDEZ-DIAZ, Institut Laue-Langevin, JINGGUANG CHENG, Materials Science and Engineering Program, University of Texas at Austin; Institute for Solid State Physics, University of Tokyo, Kashiwanoha, JOHN B. GOODENOUGH, Materials Science and Engineering Program, University of Texas at Austin — High-resolution neutron powder diffraction has been performed to study the structural evolution of the perovskite KCuF$_3$ at temperatures up to 900 K. Results of the Rietveld refinement reveal an unusual site distortion that increases as temperature increases. In contrast to the widely accepted assumption that a cooperative Jahn-Teller transition may occur at 800 K, no phase transition was observed up to 900 K. We have made a comparative study of the Jahn-Teller distortion in fluorides and oxides with variables such as temperature, pressure, and the dilution by non-Jahn-Teller active ions in these compounds.

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