

Abstract Submitted
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Ca₂Ru_{1-x}Cr_xO₄ (0 < x < 0.13): Negative volume thermal expansion via orbital and magnetic orders¹ T.F. QI, O.B. KORNETA, M. GE², L.E. DE LONG, G. CAO, Department of Physics and Astronomy, University of Kentucky, S. PARKIN, Department of Chemistry, University of Kentucky, P. SCHLOTTMANN, Florida State University — Ca₂RuO₄ undergoes a metal-insulator transition at T_{MI} = 357 K, followed by a well-separated transition to anti-ferromagnetic order at T_N = 110 K. Dilute Cr doping for Ru reduces the temperature of the orthorhombic distortion at T_{MI} and induces ferromagnetic behavior at T_C. The lattice volume V of Ca₂Ru_{1-x}Cr_xO₄ (0 < x < 0.13) abruptly expands with cooling at both T_{MI} and T_C, giving rise to a total volume expansion ΔV/V ≈ 1 %, which sharply contrasts the smooth temperature dependence of the few known examples of negative volume thermal expansion driven by anharmonic phonon modes. In addition, the near absence of volume thermal expansion between T_C and T_{MI} represents an Invar effect. The two phase transitions, which surprisingly mimic the classic freezing transition of water, suggest an exotic ground state driven by an extraordinary coupling between spin, orbit and lattice degrees of freedom.

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