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Structural and Magnetic Phase Coexistence in Oxygen Deficient Perovskites (Sr,Ca)FeO_{2.5+δ}¹ J. P. CARLO, M. E. EVANS, J. A. ANCZARSKI, J. OCK, K. BOYD, J. R. POLLICHEMI, I. A. LEAHY, W. VOGEL, A. J. VI-ES-CAS, G. C. PAPAETHYMIOU, Villanova University — A variety of compounds crystallize into perovskite and similar structures, making them versatile laboratories for many phenomena and applications, including multiferroicity, superconductivity, and photovoltaics. Oxygen-deficient perovskites ABO_x have attracted interest for use in fuel cells and related applications due to high oxygen mobility and the possibility of charge disproportionation. Vast chemical flexibility is obtained through reductions in lattice symmetry and rotation/distortion of the BO₆ octahedra, as well as ordering of oxygen vacancies. We have synthesized and studied the structural and magnetic properties of oxygen-deficient perovskites (Sr,Ca)FeO_{2.5+δ} using x-ray diffraction and Mossbauer spectroscopy. While the ideal perovskite has $\delta = 0.5$, this requires Fe⁴⁺, and hence strongly oxidizing environments. When grown in air, Fe³⁺ is favored, yielding $\delta \approx 0$. SrFeO_{2.5+δ} exhibits cubic symmetry and paramagnetism at 300K, but CaFeO_{2.5+δ} crystallizes into the orthorhombic brownmillerite structure, and is magnetically ordered at 300K. In the doped intermediaries we find coexistence of cubic/paramagnetic and orthorhombic/magnetic phases over a wide range of Ca content.

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