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Crystal Fields as a Probe of the Valence Transition in Pr-based Cobaltites D. PHELAN, S. ROSENKRANZ, Argonne National Laboratory, D.M. PAJEROWSKI, NIST Center for Neutron Research, C. LEIGHTON, University of Minnesota — Upon cooling, a unique first-order metal-insulator transition (MIT) has been observed in cobaltite perovskites at certain compositions with Pr on the A-site; this is strongly suspected as a consequence of electron transfer from Pr^{3+} ions to hybridized Co-O orbitals. Here we discuss the crystal field levels of Pr^{3+} and Pr^{4+} ions which we have investigated using inelastic neutron spectroscopy as a function of temperature for three samples: one insulating, one metallic, and one that undergoes the MIT. We show that the insulating compound, $\text{PrCoO}_{3-\delta}$, contains Pr^{3+} ions ($J=4$) whose ground state multiplet is split into nine singlets, and we extract its crystal field parameters. In the hole-doped metal, $\text{Pr}_{0.7}\text{Ca}_{0.3}\text{CoO}_{3-\delta}$, which also contains Pr^{3+} ions, the crystal field levels maintain the same energy-level structure but are noticeably broadened. The scattering from the Pr^{3+} crystal fields, though present, is diminished in the sample that undergoes the MIT ($\text{Pr}_{0.63}\text{Y}_{0.07}\text{Ca}_{0.3}\text{CoO}_{3-\delta}$), consistent with a decrease in the concentration of Pr^{3+} ; moreover, the levels are severely broadened. The experiments illustrate the inhomogeneous charge distribution that occurs around the Pr sites upon substitution.

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