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Local Electronic and Spin Structure of GdBaCo2O5.5 from X-ray Absorption Spectroscopy KYLE SHEN, DAVID HAWTHORN, DARREN PEETS, ILYA ELFIMOV, GEORGE SAWATZKY, University of British Columbia, ALEXEY TASKIN, YOICHI ANDO, CRIEPI, Japan — The family of $RBaCo_2O_{5+\delta}$ cobaltates is known to exhibit a rich variety of magnetic behavior as a function of oxygen content and temperature. We present x-ray absorption measurements on detwinned single crystals of $GdBaCo_2O_{5.5}$, where the structure is comprised of alternating rows of CoO_6 octahedra and CoO_5 pyramids. $GdBaCo_2O_{5.5}$ exhibits successive paramagnetic, ferromagnetic, and antiferromagnetic phases, and also exhibits a "spin blockade" effect upon doping. These unusual behaviors are believed to stem from the nearly degenerate spin states of the Co^{3+} ions which can potentially vary from low (S=0), intermediate (S=1), to high (S=2) spin states. Our recent x-ray absorption measurements provide the first measurements of the local electronic and spin states. Measurements of the temperature and polarization dependence of the x-ray absorption at the oxygen K edge clearly indicate an abrupt change in the orbital populations at the metal-insulator transition at T $\sim$ 360 K. We combine our spectroscopic measurements with atomic multiplet and LSDA+U calculations to provide a first insight into the true nature of the spin state transitions which govern the unusually rich magnetic properties of the $RBaCo_2O_{5+\delta}$ cobaltates.

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