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Oxygen Defect Structure in the Geometrically Frustrated Kagomé System $YBaCo_4O_{7+\delta}$: Impact on Structure and Magnetic Properties[1] S. AVCI, Bursa Technical University and Argonne National Laboratory, O. CHMAISSEM, Northern Illinois University and Argonne National Laboratory, H. ZHENG, Argonne National Laboratory, A. HUQ, Oak Ridge National Laboratory, P. MANUEL, ISIS, Rutherford Laboratory, UK, J. F. MITCHELL, Argonne National Laboratory — The RBaCo4O7 family "R-114"(where R = rare earth, Y or Ca) have been a model system due to their high oxygen affinity, significant electrochemical properties and geometric frustration, in which face-sharing tetrahedra of Co ions link to form trigonal bipyramids on a Kagomé lattice. Here we report quantitative thermogravimetric analysis (TGA), *in-situ* x-ray diffraction (XRD), high resolution synchrotron x-ray and neutron diffraction data characterizing the oxygen uptake/release phenomenon and its impacts on structure and magnetic properties of $YBaCo_4O_{7+\delta}$. We show that $YBaCo_4O_{7+\delta}$ reaches an equilibrium state with $\delta \sim 0.1$ when heated slightly above 350 ^{o}C. When heated slightly below 350 ^{o}C, it absorbs significantly more oxygen ($\delta = 1 \sim 1.1$) and shows the orthorhombic $Pbc2_1$ symmetry previously reported [O. Chmaissem et al. J. Solid State Chem. 181, 664 (2008)]. We also detected the existence of a miscibility gap that separates the $\delta = 0$ and $\delta = 0.1$ phases. In samples $\delta \geq 0.1$, excess oxygen suppresses the structural transition however, there are strong short range magnetic correlations below 100 K despite the preserved Kagomé structure.

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