Abstract Submitted
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Neutron diffraction study of quasi-one-dimensional lithium purple bronze: possible mechanism for dimensional crossover[1] JOHN J. NEUMEIER, M.S. DA LUZ, Montana State University, C.A.M. DOS SANTOS, Escola de Engenharia de Lorena - USP, B.D. WHITE, Montana State University, H.J.I. FILHO, Escola de Engenharia de Lorena - USP, J.B. LEÃO, Q. HUANG, NIST Center for Neutron Research — The crystallographic structure of quasi-1D lithium purple bronze was investigated using neutron powder diffraction at temperatures T in the range 5 K $< T <$ 295 K. Lattice parameters, atomic positions, and occupation numbers are reported. At room temperature, it has a monoclinic symmetry with space group $P2_1/m$, lattice parameters $a = 12.750(1)$ Å, $b = 5.524(1)$ Å, $c = 9.491(2)$ Å, and $\beta = 90.593(1)^\circ$. The stoichiometry was determined through chemical analysis *and* refinement of the NPD data to be $Li_{0.924}Mo_6O_{17.6}$. The bond-valence-sum method was applied to calculate the valence of each Mo ion as a function of T, which allows discussion of the mechanism by which charge is transferred between the double 1D conducting chains.

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