Abstract Submitted
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Powder neutron diffraction study of quasi-one-dimensional $\mathbf{Li_{0.9}Mo_6O_{17}}$[1] MARIO S. DA LUZ, Montana State University, C.A.M. DOS SANTOS, Escola de Engenharia de Lorena, B.D. WHITE, J.J. NEUMEIER, Montana State University, Q. HUANG, J.B. LEAO, J.W. LYNN, NIST Center for Neutron Research — The crystallographic structure of quasi-one-dimensional $Li_{0.9}Mo_6O_{17}$ was investigated by Rietveld refinement of powder neutron diffraction data at temperatures in the range 5 K $< T <$ 295 K. Structural parameters, atomic positions, occupation numbers, and isotropic thermal parameter B_{iso} will be reported. The occupancy was refined revealing a Li occupancy greater than 0.9. Bond valences sums will also be reported for various Li and Mo sites. At room temperature, the crystal was found to exhibit monoclinic symmetry with space group P21/m and lattice parameters a =12.7506(1) Å, b = 5.5242(1) Å, c = 9.4913(2) Å and β = 90.593(1)^o. Good agreement between the temperature dependence of lattice parameters and high resolution thermal expansion results* was obtained. *C. A. M. dos Santos, B. D. White, Yi-Kuo Yu, J. J. Neumeier, and J.A. Souza, Phys. Rev. Lett. **98**, 266405 (2007).

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John J. Neumeier
Montana State University

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