Abstract Submitted
for the TS4CF08 Meeting of
The American Physical Society

Negative thermal expansion in hexacyanocobaltates of divalent metals SOURAV ADAK, New Mexico State University, LUKE DAEMEN, Los Alamos Neutron Science Center, HEINRICH NAKOTTE, New Mexico State University — While many Prussian Blue analogs are known to display negative thermal expansion (NTE), few have been studied in detail. Not all compounds in this family exhibit NTE. Because it is possible to systematically vary ion size and charge in these materials, they represent an interesting playground to study NTE and possible correlations with electronic and crystal structures. By contrast with many silicates displaying NTE and in which tetrahedral units are linked with apical oxygens, the octahedral units in Prussian Blue compounds are linked with a linear cyanide ligand. This introduces more degrees of freedom in the (mostly) cubic structures. Powder samples of hexacyanocobaltates of divalent metals with general formula$M_3^{II}[Co^{III}(CN)_6]_2$ (M = Co, Cu, Mn, Ni, and Zn) were prepared via standard chemical precipitation. X-ray powder diffraction patterns were collected at room temperature (T_2= 300K) and at liquid nitrogen temperature (T_1 = 77K) to obtain an average coefficient of thermal expansion. The X-ray data were analyzed using the Rietveld refinement technique with the General Structure Analysis System (GSAS) software. All the materials studied are cubic with space group $Fm\bar{3}m$ or $F\bar{4}3m$. The thermal expansion coefficients of the five compounds are determined to be in the range 3.5 x $10^{-6}K^{-1}$ – 46.6 x 10^{-6} K^{-1}.

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Date submitted: 16 Sep 2008 Electronic form version 1.4