

Abstract Submitted  
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**Negative thermal expansion in Prussian Blue analogs** S. ADAK, H. NAKOTTE, L. DAEMEN, LANSCE (Lujan Center), LANL — While many Prussian Blue (PB) 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 PB compounds are linked with a linear cyanide ligand. This introduces more degrees of freedom in the (mostly) cubic PB structures compared to the silicates. Polycrystalline samples of PB analogs,  $M_2^{II}[Fe^{II}(CN)_6]$  and  $M_2^{III}[A^{III}(CN)_6]_2$  ( $M = Mn, Co, Ni, Cu, Zn; A = Cr, Fe, Co$ ) were synthesized via standard chemical precipitation. Variable temperature X-ray powder diffraction patterns were collected *in-situ* in the range 300-123 K to study the T-dependence of the lattice parameter and to obtain an average coefficient of thermal expansion (CTE). Lattice parameters were extracted using the Rietveld refinement technique with the General Structure Analysis System (GSAS) software. The determined average CTEs, for the compounds showing NTE behavior, are in the range  $-4.9 \times 10^{-6} K^{-1}$  to  $-39.5 \times 10^{-6} K^{-1}$  while the CTEs for the other materials showing positive TE behavior are in the range  $5.9 \times 10^{-6} K^{-1}$  –  $59.2 \times 10^{-6} K^{-1}$ .

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