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Negative thermal expansion in hexacyanoferrates(III) of divalent metals S. ADAK, New Mexico State University, L. DAEMEN, H. NAKOTTE, D. WILLIAMS — Many Prussian Blue (PB) analogs are known to exhibit negative thermal expansion (NTE) behavior. However, detail studies of the NTE behavior in these compounds and the underlying mechanism behind such behavior are often missing in the literature. It is possible to systematically vary the charge and the ion size in the PB analogs. The octahedral units in PB analogs are linked with a linear cyanide ligand. This introduces more degrees of freedom in the (mostly) cubic structures. Therefore, the PB compounds offer an interesting playground to study NTE phenomenon and its possible correlations with crystal and electronic structures. The thermal expansion behavior of five PB analogs, hexacyanoferrates(III) of divalent metals with general formula$M_3^{II}[Fe^{III}(CN)_6]_2$ (M = Mn, Co, Ni, Cu, and Zn), has been studied using X-ray powder diffraction measurements. Polycrystalline samples of the studied compounds were prepared via standard chemical precipitation. The X-ray data collected at 300 and 84 K while cooling were analyzed using the Rietveld refinement technique. The crystal structures of the materials studied are cubic with space group$Fm\bar{3}m$ or $F\bar{4}3m$. The analysis indicates the occurrence of NTE in hexacyanoferrates(III) of Co, Cu, and Zn. The NTE coefficients were found to be in the range 15 x $10^{-6}K^{-1}$ – 31 x 10^{-6} K^{-1}. The other two compounds exhibit positive thermal expansion.

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