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Thermal Expansion in 3d-Metal Prussian Blue Analogs – A Survey Study S. ADAK, NMSU, L. DAEMEN, M. HARTL, D. WILLIAMS, J. SUMMERHILL, H. NAKOTTE — We present a comprehensive study of the structural properties and the thermal expansion behavior of 17 different Prussian Blue Analogs (PBAs) with compositions $M_3^{II}[(M')^{III}(CN)_6]_2.nH_2O$ and $M_2^{II}[Fe^{II}(CN)_6].nH_2O$, where M^{II} = *Mn, Fe, Co, Ni, Cu* and *Zn*, $(M')^{III}$ = *Co, Fe* and n = 5 to 18. Temperature-dependent X-ray diffraction studies were performed in the temperature range between -150^{o}C (123 K) and room temperature. The vast majority of the studied PBAs were found to crystallize in cubic structures of space groups $Fm\bar{3}m$, $F\bar{4}3m$ and $Pm\bar{3}m$. The temperature dependence of the lattice parameters was taken to compute an average coefficient of linear thermal expansion in the studied temperature range. Of the 17 compounds, 9 display negative values for the average coefficient of linear thermal expansion, which can be as large as 39.7 x 10^{-6} K^{-1} for $Co_3[Co(CN)_6]_2.12H_2O$. All of the $M_3^{II}[Co^{III}(CN)_6]_2.nH_2O$compounds show negative thermal expansion behavior, which correlates with the Irving-Williams series for metal complex stability. The thermal expansion behavior for the PBAs of the $M_3^{II}[Fe^{III}(CN)_6]_2.nH_2O$ family are found to switch between positive (for M = *Mn, Co, Ni*) and negative (M = *Cu, Zn*) behavior, depending on the choice of the metal cation (M). On the other hand, all of the $M_2^{II}[Fe^{II}(CN)_6].nH_2O$ compounds show positive thermal expansion behavior.

S. Adak
NMSU

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