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Crystal Structures and Oxygen Position in Prussian Blue Analogs
MICHAEL BOERGERT, MANJITA SHRESTHA, New Mexico State University, LUKE DAEMEN, GRAHAM KING, Los Alamos National Laboratory, EDWIN FOHTUNG, HEINZ NAKOTTE, New Mexico State University — Prussian Blue Analogs (PBAs) are a family of compounds that crystallize in cubic structures similar to the parent Prussian Blue, $Fe_4(Fe(CN)_6)_2$. In recent years, some PBAs have attracted attention because of negative thermal expansion effects. In PBAs, other metal cations occupy the Fe^{2+} and Fe^{3+} positions of the original Prussian Blue. The 3d transition metal PBAs synthesize at compositions $M_3(M'(CN)_6)_2$.xH2O, where M and M' are the metal ions and x is the number of water molecules. The metals lie at the center of an alternating octahedral C and N framework. For some of the compounds, one finds that there are additional metal ions in the centers of the octahedral framework while for others there is evidence for defects within the octrahedrals. Moreover, PBAs typically accommodate between 10 and 20 water molecules per unit cell. In this study, neutron diffraction was used to identify the crystal structures and the location of the oxygens from the water molecules for five PBAs, namely $Co_3(Cr(CN)_6)_2$, $Co_3(Fe(CN)_6)_2$, $Cu_3(Fe(CN)_6)_2$, $Mn_3(Fe(CN)_6)_2$, and $Ni_3(Fe(CN)_6)_2$.

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