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Crystal Structure of $Ni_3^{2+}[Fe^{3+}(CN)_6]_2.nH_2O$ Prussian Blue Analogue MD MINUDDIN, SEYEDAYAT GHAZISAEED, BORIS KIEFER, HEINZ NAKOTTE, New Mexico State University — The Prussian Blue Analogue (PBA), $Ni_3^{2+}[Fe^{3+}(CN)_6]_2.nH_2O$, was previously reported to crystallize in the cubic F-43m structure. However, our Density-Functional-Theory (DFT) calculations for this PBA predicted the existence of an alternative tetragonal P-4m2 structure, which is energetically degenerate with the F-43m structure. The computations also suggested that maximum possible water molecules per formula unit is n =7. To verify our computed structure, we synthesized this PBA using the chemical precipitation method and we performed X-ray (XRD) and neutron diffraction (ND) measurements. Rietveld refinement of the XRD data satisfies the framework structure but they are insensitive to the position of light elements such as H. Rietveld refinement of ND data were also unable to solve the issue as H has high incoherent scattering cross section. To test hydrogen positions experimentally, we synthesized a deuterized sample of this PBA since D has much smaller incoherent scattering cross section compared to H for ND studies. As H_2O and D_2O have almost same bond lengths and bond angles, the same framework structure is expected for the deuterized sample. We will present the current state of our analysis of our ND data for the deuterized PBA using the Rietveld refinement package GSAS II.

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