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Probing thermal decomposition of $\mathbf{Ni_3^{+2}[Fe^{3+}(CN)_6]_2.nH_2O}$ MD MINUDDIN, New Mexico State University, ERIC NOVAC, LUKE DAEMEN, Oak Ridge National Laboratory, BORIS KIEFER, HEINZ NAKOTTE, New Mexico State University — The Prussian Blue Analogue (PBA), $Ni_3^{+2}[Fe^{3+}(CN)_6]_2.nH_2O$, has a framework structure with alternating C_6 and N_6 octahedra with the transitional metals at the octahedral centers and connected with rigid $C-N$bonds. The water molecules are located either in the framework between octahedra or on C or N defect sites. Thermal decomposition PBA is commonly inferred from the Thermogravimetric Analysis (TGA) by considering the mass loss is due to the loss of water molecules, while the framework structure remains the same. We had performed DFT calculations, and it indicates a different decomposition mechanism. To probe the decomposition, we prepared a deuterized sample as D has higher coherent scattering length than H. We performed powder neutron diffraction at different temperatures between room temperature and 600^0C. We used Rietveld refinement on the average structure and pair distribution function analysis on the local structure. Our analysis shows that at elevated temperature the framework structure is distorted, and certain bond vanishes.

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