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Elastic and inelastic neutron scattering from Prussian Blue Analogs, Fe3[Co(CN)6]2.n(H/D)2O

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Prussian Blue Analogs (PBAs) are families of cyano-bridged nanoporous open framework coordination polymers. Owing to their simple crystal structure, cubic for most of the compounds, tunable composition, compositional dependence of various properties, and because of their various potential applications, they offer an interesting playground to study various different properties and their correlation with structure and dynamics. PBAs have recently gained a huge importance due to their applications in energy technologies including energy storage, electrolysis, and thermal power generations. Importantly, PBAs are also being used as excellent cathode materials in Na- and K-ion battery technology. In addition, these materials often show negative thermal expansion (NTE) behavior which is important in its own right. Herein, we explore and report a study of structure-dynamics-properties (mainly NTE) relationship by employing elastic (diffraction) and inelastic incoherent neutron scattering (IINS) from a representative material, Fe3[Co(CN)6]2.n(H/D)2O. Simultaneous neutron diffraction and vibrational spectroscopic data were collected at VISION instrument at Spllation Neutron Source, Oak Ridge National Laboratory and were analyzed in combination with computational modeling. Our investigation revealed that the compound, when fully hydrated, shows both positive and negative thermal expansion while, interestingly, dehydrated phase of the compound shows NTE behavior only.

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