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Structural Features of Prussian Blue Analogs MICHAEL BOERGERT, New Mexico State University, EDWIN FOHTUNG, HEINZ NAKOTTE, New Mexico State University, Los Alamos National Laboratory, LUKE DAEMEN, Oak Ridge National Laboratory — Most Prussian Blue Analogs (PBAs) crystallize in cubic framework structures with alternating C or N octahedrals that contain metal ions. The vast majority of PBAs exhibit negative thermal expansion (NTE), which is of great interest for applications. A full understanding of NTE effects requires detailed knowledge of the structural features of these compounds. This study looks into X-ray diffraction patterns of single-crystalline grains of an exemplary Prussian Blue Analog, taken at the Advanced Photon Source (APS) at Argonne National Laboratory. We collected three-dimensional sets at various temperatures, and the main and lesser peaks of each data set were analyzed. The analysis provides the peak widths, peak shapes (Gaussian or Lorentzian) and peak locations, and the results were used to determine the long- and short-range features of this particular PBA.

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