

MS27-P03 | LOCAL ORDER IN CO AND MN PRUSSIAN BLUE ANALOGUES, THE 3D- Δ PDF

ANALYSIS.

Simonov, Arkadiy (ETH Zurich, Zürich, CH); Boström, Hanna (Uppsala University, Uppsala, SWE); Goodwin, Andrew (University of Oxford, Oxford, GBR)

Prussian Blue Analogues is a family of materials with the general formula $M'[M''(\text{CN})_6]_{1-x} \cdot \text{H}_2\text{O}$ where M' and M'' are transition metals. These materials are currently actively investigated due to their interesting stimuli-dependent magnetic, electronic and optical properties.

This materials are disordered, since In order to achieve the charge balance, the site containing the hexacyanometallate group $[M''(\text{CN})_6]$ is partially vacant. This disorder is important for physical properties, since it defines the internal flexibility of the structure. Up until now, only qualitative models of disorder were proposed [1-2].

In this work we will present the quantitative investigation of local correlations between the vacancies in single crystals of two members of the Prussian blue analogue family: $\text{Mn}[\text{Co}(\text{CN})_6]_{2/3} \cdot \text{H}_2\text{O}$ and $\text{Co}[\text{Co}(\text{CN})_6]_{2/3} \cdot \text{H}_2\text{O}$. The crystals show a very similar ordering pattern on the $[M''(\text{CN})_6]$ groups and vacancies, however the manganese version contains additional diffuse scattering features which are associated with the correlated displacements of the $[M''(\text{CN})_6]$ columns.

[1] Bhatt, P., Thakur, N., Mukadam, M.D., Meena, S.S. and Yusuf, S.M. (2013), J. Phys. Chem. C, 117(6), 2676-2687

[2] Chernyshov, D. and Bosak, A. (2010), Phase. Trans., 83(2), 115-122