Pressure-induced changes in the structural properties of potassium-based prussian blue analogues

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Prussian blue analogues (PBAs) are coordination compounds comprising a metal cyanido framework of general formula $A_xM[M'(CN)_6]_y \cdot nH_2O$ with A representing alkali metals and M/M′ representing transition metals. The structure consists of transition metal centres connected through cyanide bridges in an octahedral arrangement. PBAs have generated a lot of interest due to the large degree of structural freedom in this family of compounds, including A, M, M', or hydration, allowing for variable properties that are ideal for a broad range of applications, such as multiferroic materials [1]. Multiferroic materials combine switchable electric and magnetic order, and carry immense potential for applications in data storage systems [2]. Polar symmetry is required for multiferroic behaviour. In $A_xMn[Co(CN)_6]_y \cdot nH_2O$, phase transitions to polar symmetry appear under pressure, stemming from a hybrid improper ferroelectric mechanism [3, 4]. Hybrid improper ferroelectricity means the spontaneous polarisation induced by two different structural distortions collectively working together, which is here the tilting and the A-site cation order. In this study, we present the hydrothermal synthesis of the potassium-based Prussian blue analogue $K_xMn[Co(CN)_6]_y$ at various pressure points. We shed light on pressure-dependent phase transitions and analyse the respective structural properties of these phases.

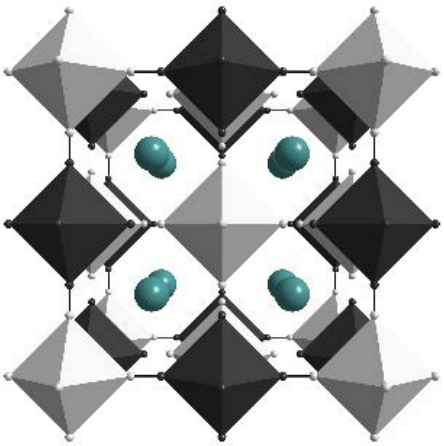

Figure 1. Excerpt of the crystal structure of $K_xMn[Co(CN)_6]_y$.

[1] Scott, J. F. (2007). *Nat. Mater.* **6**, 256−257.

[2] Scott, J. F. (2007) *Science*. **315**, 954−959.

[3] Benedek, N. A. & Fennie, C. J. (2011) *Phys. Rev. Lett.* **106**, 107204.

[4] Boström, H. L. B., Collings, I. E., Daisenberger, D., Ridley, C. J., Funnell, N. P., Cairns, A. B. (2021) *J. Am. Chem. Soc.* **143**, 3544−3548.