

Structure-magnetic property correlations in metal-formate frameworks at high pressure [Abstract]

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MS17-P02 | STRUCTURE–MAGNETIC PROPERTY CORRELATIONS IN METAL–FORMATE FRAMEWORKS AT HIGH PRESSURE

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Magnetic metal–organic frameworks (MOFs) have attracted increasing interest due to their capabilities of coupling magnetism with other properties, such as ferroelectricity, porosity, and optical activity [1]. The structural flexibility and responsive nature of MOFs mean that significant changes in their magnetic properties could be achieved upon their exposure to external stimuli. However, few guidelines exist to tune and improve their magnetic properties. High-pressure investigations are particularly useful as they allow changes in the magnetic properties to be related to structural variations without additional electronic effects that are present upon chemical substitutions.

The family of protonated amine or ammonium templated metal formates display a range of interesting physical properties, such as ferroelectricity, antiferromagnetism, multiferroicity, and have a rich chemical diversity. Here, we investigate the structural and magnetic properties of ammonium metal formates [2], $[\text{NH}_4][\text{M}(\text{HCOO})_3]$, for $\text{M} = \text{Mn}^{2+}$, Fe^{2+} , Ni^{2+} , at high pressure up to 2.5 GPa and low-temperature conditions by use of single-crystal X-ray diffraction and magnetisation measurements. We find that the overall magnetic behaviour of each phase upon compression was not only dependent on the structural distortions but also on the electronic configuration of the metal cation [3].

[1] G. Rogez *et al.*, *Angew. Chem. Int. Ed.* **2010**, 49, 1921–1923.

[2] G.-C. Xu *et al.*, *J. Am. Chem. Soc.* **2011**, 133, 14948–14951.

[3] I. E. Collings *et al.*, *Phys. Chem. Chem. Phys.* **2018**, 20, 24465–24476.