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Spin-density studies of the multiferroic metal–organic compound $[\text{NH}_2(\text{CH}_3)_2][\text{Fe}^{\text{III}}\text{Fe}^{\text{II}}(\text{HCOO})_6]$

Metal–organic frameworks combining two or more properties have been the focus of interest of several research groups in the last few decades. A good approach to achieve this combination has been the design of perovskite-like metal–organic frameworks where a three-dimensional network made of metallic centres linked through organic ligands, which presents magnetic order, also accommodates counterions responsible for electric order. One of these examples is the mixed-valence iron(II)–iron(III) formate compound $[\text{NH}_2(\text{CH}_3)_2][\text{Fe}^{\text{III}}\text{Fe}^{\text{II}}(\text{HCOO})_6]$.

Previous results revealed that upon cooling, the magnetic moments of the Fe(II) and Fe(III) sublattices do not order simultaneously: the magnetization of the Fe(II) sublattice increases faster than that of the Fe(III) sublattice because of the larger value of the saturation magnetization of the latter.[1] Unpolarized neutron diffraction measurements at 2 K with no external field revealed some discrepancies in the saturation value of the magnetic signal on the Fe(III) sites and in the ferromagnetic moment along the *c* axis. These discrepancies could be related to the actual distribution of magnetic moment, since unpolarized neutron diffraction gives information on the magnetic moment localized only on the magnetic ions. Polarized neutron diffraction allows an analysis of the magnitude of the spin density over magnetic and nonmagnetic ions (the organic ligand and the counterion), which can give a clue to explain the low saturation on the Fe(III) sublattice and the correlation with the physical measurements.

The present study also contributes to the understanding of the magneto-electric behaviour of this compound, giving insight into the role of metal disorder in the origin of the structural phase transition, which is responsible for its antiferroelectric order, and into the influence of spin-density delocalization on its magneto-electric properties, allowing a discussion of the alternative explanations given so far for its electric properties at low temperature. [2]

References:

1. Cañadillas-Delgado, L., Fabelo, O., Rodríguez-Velamazán, J. A., Lemee-Cailleau, M. H., Mason, S. A., Pardo, E., Lloret, F., Zhao, J. P., Bu, X. H., Simonet, V., Colin, C. V. & Rodríguez-Carvajal, J. (2012). *J. Am. Chem. Soc.* 134, 19772–19781.
2. Cañadillas-Delgado, L., Fabelo, O., Rodríguez-Velamazán, J.A., Stunault, A., Zhao, J., Bu, X. & Rodríguez-Carvajal, J. (2020) *IUCrJ*, 7, 803-813.

Primary author: CANADILLAS-DELGADO, laura (Institut Laue Langevin)

Co-authors: STUNAUULT, Anne (ILL); RODRIGUEZ-VELAMAZAN, J. Alberto (ILL); FABELO, Oscar (ILL); RODRIGUEZ-CARVAJAL, juan (ILL)

Presenter: CANADILLAS-DELGADO, laura (Institut Laue Langevin)

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