

## Microsymposium

MS106.O03

### *Spin Density Distribution in a MOF presenting electric and magnetic order*

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One of the main features of molecular compounds is the possibility of combining different properties in a synergic way giving a multifunctional material. Here we will discuss the case of a compound combining electric and magnetic order, thus giving a “multiferroic” molecular material. The disorder-order of the dimethylammonium molecule in the Iron(II)-Iron(III) system  $[\text{NH}_2(\text{CH}_3)_2\text{n}[\text{Fe}^{\text{III}}\text{Fe}^{\text{II}}(\text{HCOO})_6]\text{n}]$  is in the origin of the observed electric transition from paraelectric to antiferroelectric. In combination with the mentioned electric properties, this compound shows also magnetic order in the form of Néel N-Type ferrimagnetism [1]. The structure of  $[\text{NH}_2(\text{CH}_3)_2\text{n}[\text{Fe}^{\text{III}}\text{Fe}^{\text{II}}(\text{HCOO})_6]\text{n}]$  has been characterized by means of neutron diffraction at VIVALDI and D19 instruments at Institut Laue-Langevin (ILL, Grenoble, France), where a crystallographic phase transition was observed from the high temperature structure [P-31c;  $a = b = 8.2550(12)$  and  $c = 13.891(3)$  at room temperature] to a lower symmetry one [R-3c;  $a = b = 14.2600(17)$  and  $c = 41.443(8)$  at low temperature]. On the other hand, the magnetic behaviour of this compound can be described as a result of two sublattices anti-ferromagnetically coupled, containing different spin carriers  $\text{Fe}^{\text{III}}$  and  $\text{Fe}^{\text{II}}$ , respectively, with an ordering temperature of 37 K, and which are responsible of the different magnetic behaviours at low temperature.[2] The different spins of the neighbouring ions [ $S = 5/2$  and  $S = 2$ ] result in a ferrimagnetic state. Polarized neutron diffraction measurements aimed at clarifying the spin density map in order to understand the influence of the counter ion in the magnetic properties were carried out at D3 instrument (ILL). Measurements of the flipping ratios were performed with magnetic field of 9 Tesla at 45K, over the magnetic ordering temperature. The results point to an unusual weak spin density located around the counterions which suggests a non-negligible role in the magnetic behavior for the amine group.

[1] L. Cañadillas-Delgado, O. Fabelo, J.A. Rodríguez-Velamazán, et al. *J. Am. Chem.Soc.* 2013, 134, 19772, [2] J-P. Zhao, B-W. Hu, F. Lloret, et al. *Inorg. Chem.* 2010, 49 10390

**Keywords:** Spin-Density, Polarized neutrons, Molecular multiferroics