Considerable attention is currently focused on metal-organic polymers combining two or more functionalities, e.g., conductivity and magnetism, magnetic and optical properties, porosity and magnetism. The inclusion of two different metallic atoms into the niccolite-like structure framework have led to the formation of isostructural compounds of formulae [NH2(CH3)2]n[M(II)Fe(III)(HCOO)6]n with M(II) = Fe(1), Co(2) and Mn(3).

The nuclear characterization of these compounds has been done combining high resolution neutron diffraction together with synchrotron X-ray diffraction at 45K.

In compound 1 neutron studies show a sequence of phase transition involving nuclear transformation as well as a long range magnetic order. The nuclear phase transition involves an ordering of the NH2(CH3)2 countercation within the cavities framework which is related with a change in the electric behaviour from paraelectric to antiferroelectric.[1] However, in compounds 2 and 3, multipattern refinements combining X-rays and neutron radiation, permit the localization of the hydrogen atoms of the [NH2(CH3)2] counter ions, and discards the occurrence of a structural phase transition.[2] Below TN, the magnetic order in these compounds vary from an antiferromagnetic behaviour with a weak spin canting for compound 3 to a ferrimagnetic behaviour for 1 and 2 compounds, due to the competition of the different magnetic moments present in each sublattices (the different spin state involved in those complexes are S = 5/2, for Fe(III) and Mn(II) while it is 3/2 and 2 for Co(II) and Fe(II), respectively).

Neutron studies using single crystal and powder diffraction techniques have been carried out at Institut Laue Langevin (Grenoble, France) to elucidate the different magnetic behaviour present in these compounds.


Keywords: Neutron diffraction, multiferroic molecular compounds, formate compounds