Experimental report

07/08/2019

Proposal: **CRG-2557** **Council:** 4/2018

Title: Exploring the magneto-structural correlations on double salt magneticionic liquids: Dimim(Fe(ClxBr1-x4)) (0<x<1)

Research area:

This proposal is a continuation of CRG-2473

Main proposer: **Palmerina GONZALEZ IZQUIERDO**

Experimental team: Palmerina GONZALEZ IZQUIERDO
Oscar Ramon FABELO ROSA
ruben PEREZ AGUIRRE
Fabio SCE

Local contacts: Oscar Ramon FABELO ROSA

Samples: (1.3-dimethylimidazolium)[Fe(ClxBr1-x)4]

Instrument	Requested days	Allocated days	From	To
D1B	3	3	05/10/2018	08/10/2018

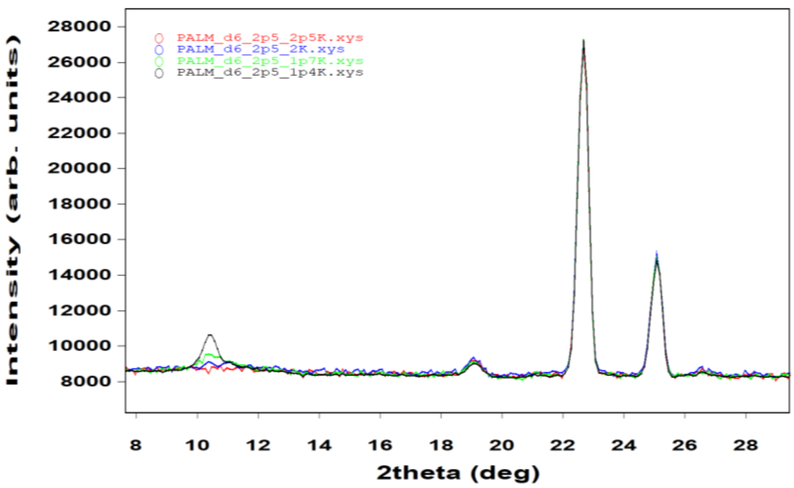
Abstract:

Report for the experiment at D1B 5-8/08/2018 proposal CRG-2557

The samples measured during this experiment have the general formula (dimim)[$Fe(Br_xCl_{1-x})_4$] (dimim=1,3-dimethylimidazolium) with *x* ranging from 0.025 to 0.75. From now on, they will be referred in the figures with the code PALM_d6_X_T (where X is the percentage of bromide and T is the temperature).

The samples with low and high bromide content show magnetic ordering at low temperature, as can be seen in Fig. 1, where the evolution of the magnetic peak for the samples with 2.5% and 75% of bromide is shown. The magnetic peak for the sample with 2.5% of bromide disappears at a lower temperature than the sample with 75% of bromide.

a)



b)

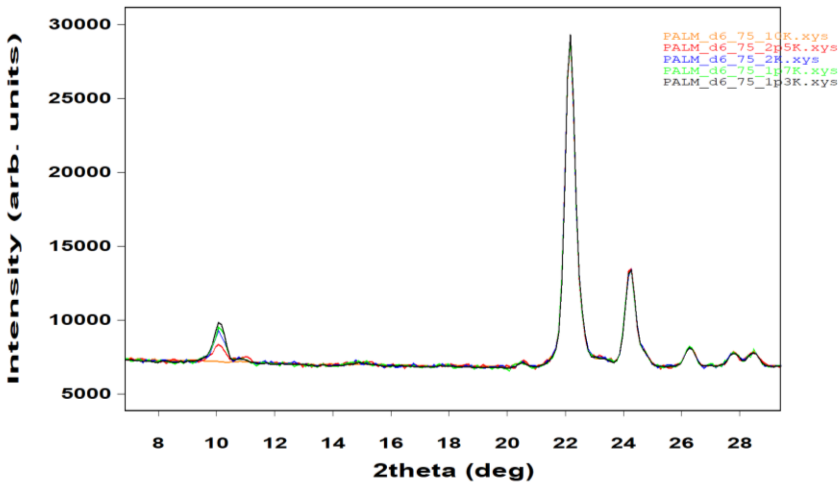
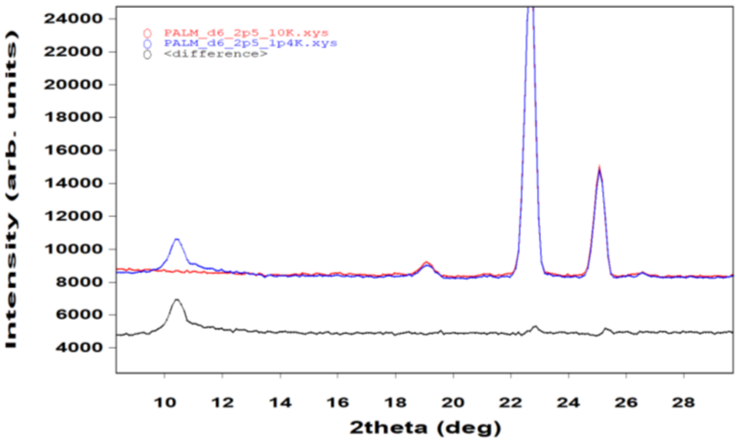


Figure 1: diffraction patterns of the sample with 2.5% of bromide (a) and 75% of bromide (b) at 1.4 (black), 1.7 (green), 2 (blue) and 2.5 (red) and 10 K (orange).

Furthermore, the lower and higher concentrations of bromide present different magnetic peaks, indicating the existence of two different magnetic structures. This can be better observed in Fig. 2, where the difference patterns between the ordered and paramagnetic phase are represented.

a)



b)

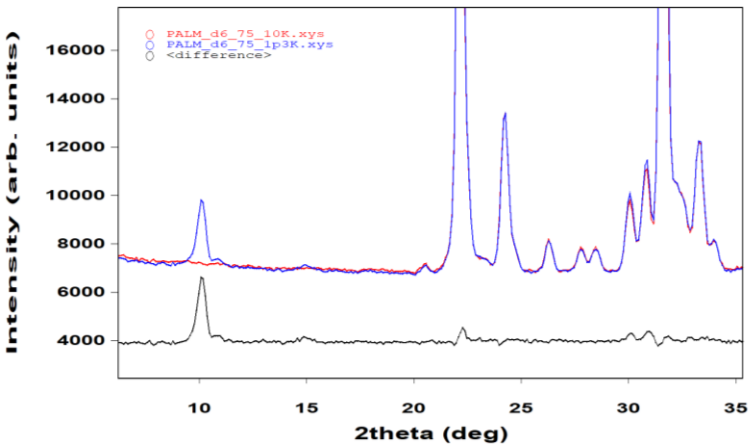


Figure 2: diffraction patterns of the sample with 2.5% of bromide (a) and 75% of bromide (b) at 1.3 (blue) and 10 K (red). The difference pattern between the aforementioned patterns is represented in black.

In Fig. 3, the diffraction patterns of all the samples at 1.3 K are shown. As it can be observed, the magnetic peak disappears apart from 15% of bromide and reappears again around 50%, which is in agreement with the specific heat measurements. This could be due to the appearance of a mixture of phases and magnetic frustration.

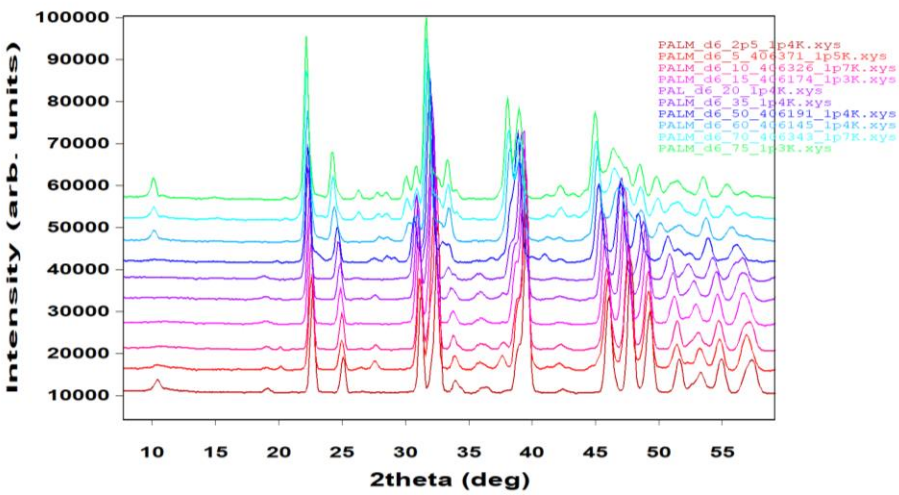


Figure 3: diffraction patterns for all the concentrations of bromide at 1.3 K. From dark red to green: lower to higher ratio Br^{-}/Cl^{-}.

We also measured temperature ramps heating from 10 to 220 K, shown in Fig. 4. No phase transition is observed for 5 and 50% of bromide. For 75%, nevertheless, the thermodiffractogram shows the merging of several peaks when heating, indicating a smooth change of structure, which is not solved yet.

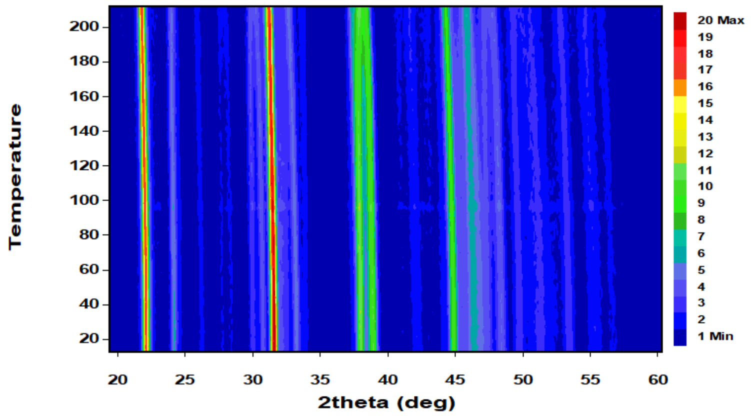


Figure 4: thermodiffractogram from 10 to 220 K for 75% content of bromide.

The Rietveld refinement of the sample with 35% of bromide to the low temperature structure of the chloride parent is shown in Fig. 5. The cell parameters, atomic positions (with distance restraints), thermal parameters and the occupation of the chloride and bromide positions were refined. The obtained R_{Bragg} is 4.54, which is a reasonably good fit to the data. Appart from 50% of bromide, this crystal structure does not fit anymore. This can be due to a mixture of phases or the appearance of a new phase. Single crystal neutron diffraction data is necessary to solve this structure.

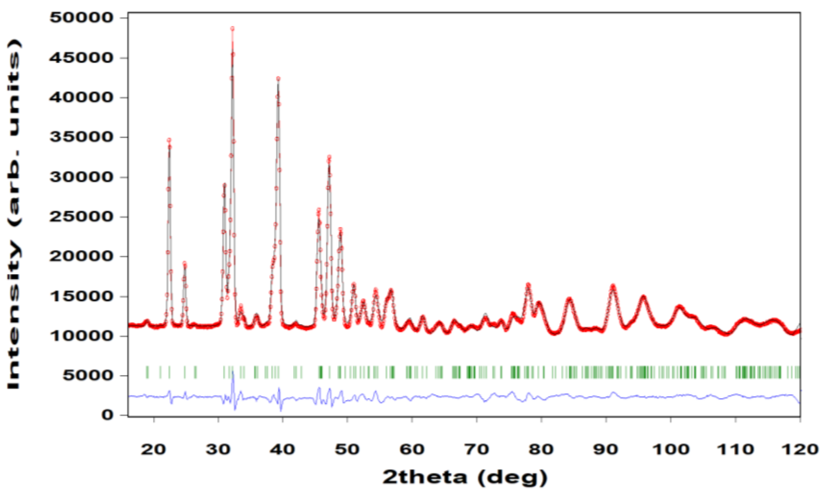


Figure 5: Rietveld refinement (black line) to the diffraction data (red points) at 1.4 K for the simple with 20% of bromide.