

Experimental report

14/03/2021

Proposal: 5-12-341

Council: 10/2018

Title: Crystal structure determination of the (trimim)[FeBr₄] hybrid halometallate compound

Research area: Materials

This proposal is a new proposal

Main proposer: Palmerina GONZALEZ IZQUIERDO

Experimental team: Palmerina GONZALEZ IZQUIERDO

Laura CANADILLAS DELGADO

ruben PEREZ AGUIRRE

Local contacts: Laura CANADILLAS DELGADO

Samples: C₆H₁₁N₂FeBr₄

Instrument	Requested days	Allocated days	From	To
D19	8	5	29/08/2019	04/09/2019
D9	12	0		

Abstract:

In recent studies, we have found that imidazolium magnetic ionic liquid based on tetrahaloferrate anions display very interesting magnetic and dynamic phenomena. Now, we synthesized the compound trimim(FeBr₄) (trimim: 1,2,3-trimethylimidazolium), which shows three-dimensional magnetic order at low temperatures. In order to solve the magnetic structure, it is necessary to know the nuclear structure. The structure obtained by previous single-crystal X-Ray and powder synchrotron X-Ray diffraction does not fit the powder neutron diffraction data acquired in the D1B instrument, possibly due to the reorientation of the imidazolium rings below 160 K. In order to solve the structure at low temperatures, we will grow crystals suitable for single-crystal neutron diffraction. With this objective, we kindly apply to 8 days on D19 to carry out high resolution single-crystal neutron diffraction or, alternatively, 12 days in D9.

Published results in:

- **J. Mol. Liq.**, 2021, 115716 <https://doi.org/10.1016/j.molliq.2021.115716>