Experimental report

14/03/2021

Proposal: 5-12-347 **Council:** 4/2019

Title: Structural characterization of theorder-disorder transition in a novel quinuclidine-based halometallatecompound: (quinuclidine)[FeCl4]

Research area: Physics

This proposal is a new proposal

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Samples: C7H13NFeCl4

Instrument	Requested days	Allocated days	From	To
D19	9	6	21/01/2020	28/01/2020
D9	16	0		

Abstract:

Quinuclidine-based halometallate compounds display very interesting dynamic phenomena as a consequence of the high mobility of the quinuclidine-based countercations. In this proposal we pretend to deep study the crystal structure of(quinuclidine)[FeCl4] compound. This compound presents a structural order-disorder transition which is related with an electric phase transition, similar to those previously observed in divalent- and monovalent cation-containing compounds. In order to survey the crystal structure as function of the temperature, we ask for the Laue diffractometer CYCLOPS. Based on the CYCLOPS results, accurate structural models at selected temperatures will be determine using the monochromatic D19 or D9 single crystal neutron diffractometers. Our main objective is determine the influence of H-bonds, which should be the final responsible of the blocking of the quinuclidine counterions in the low temperature phase.

Published results in:

- ***J. Mater. Chem. C***, 2020,**8**, 11389-11398 **https://doi.org/10.1039/D0TC02341H**