Synthesis and Physico-Chemical Characterization of Novel Organic-Inorganic Hybrid Halometallate Compounds

Mme Palmerina GONZALEZ IZQUIERDO (ILL, 71 Av. des Martyrs, , 38000 Grenoble ())

Abstract

Hybrid organic-inorganic materials offer exciting possibilities for advanced functionalities due to their combined properties. In particular, halometallate complexes exhibit interesting thermal, ferromagnetic, ferroelectric and ferroelastic properties. Among them, tetrahaloferrate(III) complexes are particularly attractive due to their magnetic behaviour. Their crystal structures arise from a complex interplay of forces, comprising hydrogen bonding and other interactions. Furthermore, these materials exhibit many phase transitions due to dynamic rearrangements of their organic parts. Research in this area requires a multidisciplinary approach involving synthesis, structural characterization, and the study of physicochemical and magnetic properties.

During my thesis at the Laue-Langevin Institute, France, in collaboration with the University of Cantabria, Spain, my scientific interests were focused on two main areas, involving the synthesis and characterization of over 20 compounds:

• Impact of Cation and halogen type: Initially, my research explored the influence of cation size, symmetry, and halogen type (Cl or Br) on the properties of materials containing imidazolium-based cations and FeX? anions. This study aimed to establish a clear link between cation and halogen design and the resulting material's behaviour.

• Exploring Plastic-Ferroelectric Hybrids: The second part of my research focused on hybrid materials that combine plastic and polar/ferroelectric phases by synthesizing and characterizing quinuclidinium-based compounds with FeCl?.

Employing a suite of X-ray and neutron diffraction techniques, including single-crystal, powder, and synchrotron experiments, we elucidated the crystalline and magnetic structures of the compounds from their melting point down to 2 K. Notably, we were able to precisely locate the hydrogen atoms and determine their role in the structures. This comprehensive structural analysis, complemented by characterization of various physicochemical properties (melting point, electrical and magnetic behavior, DSC, FT-IR, etc.), provides a profound understanding that is key to designing novel magnetic and ionic materials.