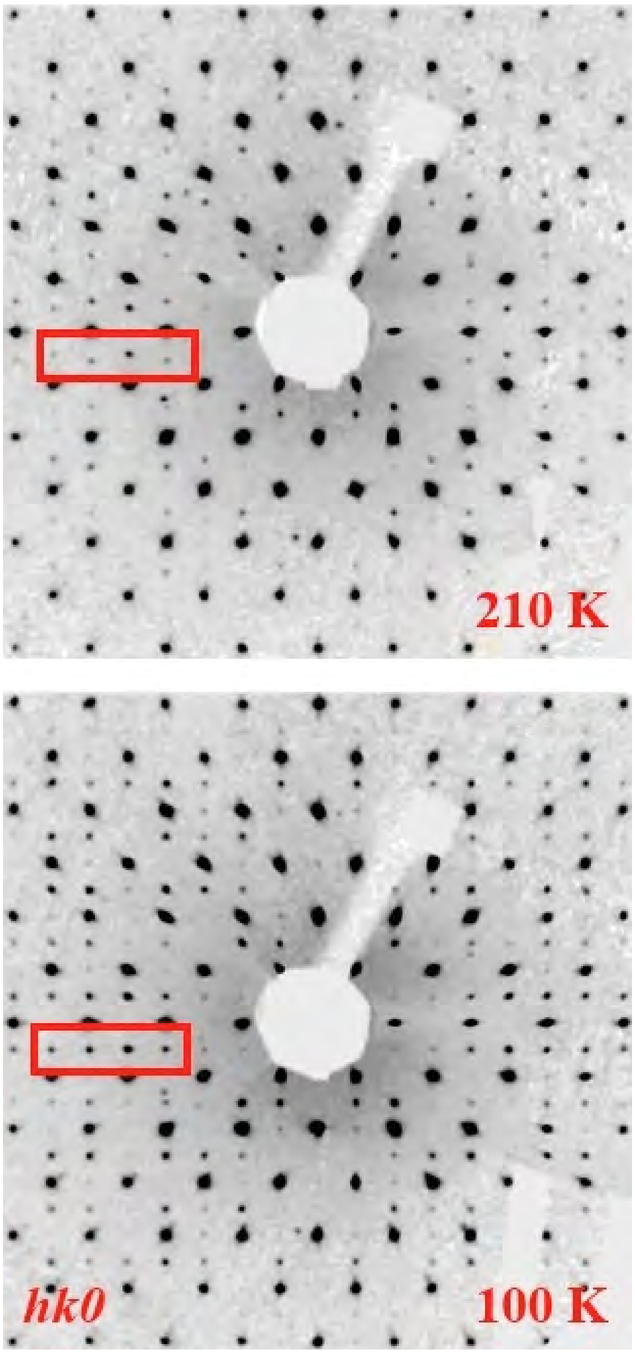

References:

[1] Bond, A. D. (2012). CrystEngComm. 14, 2363-2366.
[2] Chalker, J. M. , Thompson, A. L. & Davis, B. G. (2010). Organic Syntheses, 87, 288–298.
[3] Kim, Y., Mckinley, E. J., Christensen, K. E., Rees, N H., & Thompson, A. L. (2014). Cryst. Growth Des., 14, 6294-6301.

Keywords: Modulation, Barluenga's Reagent, Variable Temperature

MS28 Magnetic order: methods and properties

Chairs: Dr. Francoise Damay, Prof. José L. García-Muñoz

MS28-O1

On the symmetry of incommensurate magnetic structures

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The concept of symmetry in materials science trascends the role of being just a mere mathematical or geometrical property. In general, the symmetry of a crystal, within a certain thermodynamical phase, is an intrinsic physical property of the phase (phase transitions can occur without a symmetry change, but a symmetry change cannot happen without a phase transition!). In this sense, the symmetry of a crystal can be considered a thermodynamical property, which will be preserved by any possible physical atomistic mechanisms that may be active in the system as long as no phase transition occurs.

The symmetry of aperiodic crystals (structures that are ordered, but lack periodicity), is given by the so called superspace symmetry groups. As required of any well-defined generalized symmetry, these symmetry groups satisfy the above mentioned physical condition of being an intrinsic property that is necessarily preserved within a thermodynamical phase.This generalized symmetry formalism was introduced in the seventies to describe the symmetry properties of incommensurately modulated crystals, and in the next decade was further extended and applied to quasicrystals. Nowadays the formalism is fully established, and since decades superspace groups are used in a routinary and systematic way to characterize incommensurate and quasicrystalline structures.

Although the superspace formalism is easily extensible to incommensurate magnetic structures, its application to magnetic systems has remained scarce until recently. Only in the last years the development of specially adapted computer tools, and in particular, the extension of the JANA refinement program to magnetic structures has changed the situation. Using these freely available tools, superspace symmetry formalism can now be applied and this allows an efficient and rigorous description of incommensurate magnetic structures making full use of their symmetry. An additional step in this direction has been the development in the Bilbao Crystallographic Server of a small database of such structures (www.cryst.ehu.es/magndata), where the magnetic superspace group of each structure have been identified and their efficient decription using this symmetry group is shown in detail.

In this talk I will review the concepts of magnetic superspace symmetry and its application. The relation with the traditional representation method will be discussed, stressing their complementarity. Some examples retrieved from the mentioned database will help to show how representation analysis and superspace symmetry can be combined to achieve an optimal enumeration of possible physically-distinct incommensurate magnetic orderings and to obtain a detailed unambiguous rigorous characterization of magnetically modulated structures.

Keywords: incommensurate magnetic structures, supespace symmetry, magnetic symmetry

MS28-O2

Complex magnetic structure of the swedenborgite $CaBa(Co_3Fe)O_7$ derived by unpolarized neutron diffraction and spherical neutron polarimetry

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The magnetic swedenborgites, i.e. structural homologues to the hexagonal mineral $SbNaBe_4O_7$ (Refs. [1,2]), contain kagome layers with several different, similarly strong, competing spin interactions, which lead to a wide variety of ground states including chiral spin liquids), spin-glasses and long-range antiferromagnetic order. The slight structural distortions away from the hexagonal symmetry release the geometric frustration and the nature of the distortion determines the ground state. As the spins are Heisenberg-like, a Néel order is not expected unless a significant magnetic coupling between the kagome layers is at hand, which is mediated by triangular layers in-between. Here we present an extensive study on the orthorhombic compound $CaBa(Co_3Fe)O_7$ combining powder and single-crystal neutron diffraction as well as spherical neutron polarimetry (SNP). A detailed analysis of the possible irreducible representations and the magnetic structure factors in combination with the observed polarization matrices of special reflections gave clear indications concerning the magnetic symmetry. The complex situation with the presence of three structural twins and four magnetic domains (two orientational and two chiral domains) was tackled with the development of a unique software, Mag2Pol [3], which permits the refinement of a magnetic structure model including domain populations to integrated intensity and SNP data simultaneously. We could therefore derive an interesting magnetic structure of magnetic superspace symmetry P2'_1, which differs from any other member of the swedenborgite family, but which can be mapped onto the classical sqrt(3) x sqrt(3) structure of a kagome lattice. The resulting spin structure indicates an important interplay between the kagome and the triangular layers of the crystal structure.

References:

[1] Aminoff, G. (1924). Z. Kristallogr. 60, 262
[2] Aminoff, G. & Blix, R. (1933) Kgl. Sv. Vet. H. 11, 3
[3] N. Qureshi, arXiv:1801.08431.

Keywords: magnetic structure, neutron diffraction, spherical neutron polarimetry