MS25. Magnetic structures

Chairs: Oksana Zaharko, Wieslawa Sikora

MS25-O1 Symmetry-based computational tools and databases for magnetic crystallography in the Bilbao Crystallographic Server

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A deeper understanding of any magnetic ordering and its consequences requires a full characterization of the symmetry break involved. Thus, the assignment of a symmetry group (magnetic space or superspace group for a commensurate or incommensurate magnetic phase, respectively), is a basic step for the prediction and understanding of the magneto-structural properties of any magnetic phase. However, it was only in 2010 that the first computer readable listings of magnetic space groups were published, and about the same time the existing software for incommensurate structures, based in the superspace formalism, was extended to magnetic systems. These breakthroughs have been the basis for the development of novel computational tools that allow the systematic application of symmetry arguments in the study of magnetic structures. In this talk we present those recently made available in the Bilbao Crystallographic Server (www.cryst.ehu.es).

In general, the knowledge of the symmetry of the paramagnetic phase and the propagation **k**-vector(s) is sufficient to restrict the possible magnetic symmetries of a magnetic phase to a limited set. Generic magnetic structures complying with each of these symmetries can be constructed, and they can be taken as possible alternative models to be tested. The group-subgroup relations introduce an obvious hierarchy among them that can be exploited. These models can be retrieved and communicated for refinement, visualization, etc., through files in a format (magCIF), which is a direct extension of the CIF format. This is the framework of the magnetic section in the Bilbao Crystallographic Server. This approach complements and goes beyond the traditional representation method, and in this talk we present by means of various examples its capabilities. We show how the user can obtain online information about every magnetic space group (MGENPOS, MWYCKPOS, MAGNEXT), identify a magnetic space group from its symmetry operations given in an arbitrary setting (IDENTIFY MAGNETIC GROUP), derive the possible magnetic space groups for a given set of propagation vectors (MAXMAGN, k-SUBGROUPSMAG) or generate a magnetic structure model complying with a chosen magnetic space group (MAXMAGN, MAGMODELIZE). We also present MAGNDATA, a freely available online database with more than 300 magnetic structures, both commensurate and incommensurate, which are described unambiguously using magnetic symmetry, and can be retrieved in the form of magCIF files.

Keywords: Bilbao Crystallographic Server, Magnetic Crystallography, Magnetic Structures Database, Magnetic Symmetry Software