

Poster Presentation

MS90.P16

A collection of magnetic structures with cif-like files as a database seed

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We report the release within the Bilbao Crystallographic server [1] of a webpage providing detailed quantitative information on a representative set of published magnetic structures. Under the name of MAGNDATA (www.cryst.ehu.es/magndata) more than 140 entries are available. Each magnetic structure has been saved making use of magnetic symmetry, i.e. Shubnikov magnetic groups for commensurate structures, and magnetic superspace groups for incommensurate ones. This ensures a unified communication method and a robust and unambiguous description of both atomic positions and magnetic moments. The origin and main crystallographic axes of the parent phase are usually kept, with the cost of often using a non-standard setting for the magnetic symmetry. The magnetic point group is also given, so that the allowed macroscopic tensor properties can be derived. The fact that magnetic structures are being described according to various methods, often with ambiguous information, has forced an elaborate interpretation and transformation of the original data. For this purpose the freely available internet tools MAXMAGN [1] and ISODISTORT [2] have been our essential tools. Most of the analyzed structures happen to possess maximal magnetic symmetries within the constraints imposed by the magnetic propagation vector, and the relevant model could be derived in a straightforward manner using MAXMAGN [1]. In a few cases a lower symmetry is realized, but then it corresponded to one isotropy subgroup of one or several irreducible representations (irreps) of the paramagnetic grey space group, and ISODISTORT [2] could be applied to model the structure. Although the structure description is done using magnetic groups, the active irrep(s) are also given in most cases. The entries of the collection can be retrieved in a cif-like format, which is supported by internet tools as STRCONVERT [1] and ISOCIF [2], the visualization program VESTA [3], and some refinement programs (JANA2006, FULLPROF). Each entry also includes Vesta files that allow the visualization of a single magnetic unit cell.

[1] M. I. Aroyo, A. Kirov, C. Capillas, J. M. Perez-Mato & H. Wondratschek, *Acta Cryst.* A62, 115-128 (2006). (www.cryst.ehu.es), [2] B. J. Campbell, H. T. Stokes, D. E. Tanner, and D. M. Hatch, *J. Appl. Cryst.* 39, 607-614 (2006). (iso.byu.edu), [3] K. Momma and F. Izumi, *J. Appl. Crystallogr.*, 44, 1272-1276 (2011). (jp-minerals.org/vesta)

Keywords: database of magnetic structures, magnetic ordering, magnetic materials