[MS35-P04] Maximal Magnetic Groups for a given propagation vector in the Bilbao Crystallographic Server: Applications.

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A principle of symmetry maximization usually underlies the phases resulting from a symmetry-breaking phase transition. The symmetry of a stable distorted phase is often given by one of the maximal symmetry groups compatible with the transition mechanism. In the case of single-k magnetic structures, the propagation vector of the magnetic order is rather easy to identify, and the necessary compatibility with this modulation vector drastically limits the possible spin arrangements of maximal symmetry. We have implemented in the Bilbao Crystallographic Server (www.cryst.ehu.es) a new tool, called MAXMAGN, which provides them. The program determines for any space group (associated with the paramagnetic phase) and a given (single) commensurate propagation vector all possible magnetic (Shubnikov) space groups of maximal symmetry, discarding the grey ones (type II). The ouput is organized in such a way that it can be systematically applied to identify and analyse all possible alternative spin models. The general extinction rules for each case can be seen through a direct link to MAGNEXT [1]. If the structure of the paramagnetic phase is provided in a cif format, a *cif-like* file can be obtained for each of the alternative symmetry-constrained magnetic structures, which can then be used in the program ISODISTORT [2] for mode analysis, in the refinement program JANA2006 [3], or in the structure editor STRCONVERT (in the Bilbao server) for graphical representations using VESTA [4]. Both a standard setting or one adapted to the unit cell of the paramagnetic phase can be used. Some examples of application will be given, showing the predictive power of the method for multiferroic behaviour. In the simplest cases, this approach is fully equivalent to the so-called representation analysis, as the assignment of a magnetic space group introduces the same constraints as the so-called basis functions for a single one-dimensional irreducible representation (irrep) of the parent space group. But in the case of multidimensional irreps, the assumption of a maximal symmetry implies in general additional restrictions, as the active irrep basis functions must be constrained to special directions within the irrep space. All maximal magnetic groups for a given propagation vector coincide in fact with so-called isotropy magnetic subgroups (or epikernels) associated with special (1-dim) directions of the magnetic order parameter. The reverse is however not true; for space groups with some three-fold axis there can exist isotropy magnetic subgroups for specific 1-dim directions that are not maximal in the sense defined above. But these possible lower symmetries can be readily derived from the maximal ones.

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