MAGNDATA, the database of magnetic structures in the Bilbao crystallographic server, reaches 2,000 entries

J.M. Perez-Mato¹, E. S. Tasci², G. Madariaga³, L. Elcoro³, G. de la Flor⁴, M. I. Aroyo³, J. Gabirondo-Lopez³

¹Facultad de Ciencia y Tecnologia, Universidad del Pais Vasco, UPV/EHU, Apdo. 644, 48080 Bilbao, Spain. ²Department of Physics Engineering, Hacettepe University, Ankara 06800, Turkey. ³Departamento de Fisica, Universidad del Pais Vasco UPV/EHU, Leioa, Spain. ⁴Institute of Applied Geosciences, Karlsruhe Institute of Technology, Karlsruhe, Germany.

jm.perezmato@gmail.com

Keywords: Magnetic structures, Database, Magnetic symmetry, Bilbao Crystallographic Server

Back in 2014, we started to collect published magnetic structures and made them available in the Bilbao Crystallographic Server (BCS) within the program named MAGNDATA. Based on the thesis work of Samuel V. Gallego, this program accumulated by 2016 about 400 magnetic structures, all described under a standardized methodology using either magnetic space groups (MSGs) or magnetic superspace groups (MSSGs) depending on the structure being commensurate or incommensurate [1,2]. The build-up of this incipient database of magnetic structures was possible thanks to the design of the magCIF file format, which under the auspices of the Commission on Magnetic Structures of the IUCr was being developed at this time by a team headed by Branton J. Campbell. This extension of the CIF (Crystal Information Framework) dictionary, formally approved by the IUCr in 2016, is a natural generalization of the CIF format for non-magnetic structures. It uses in a standardized way, analogous to that employed in ordinary crystallography, the symmetry constraints of the magnetic group to produce a simple and unambiguous description of the magnetic structure. The listing of the magnetic moments (and their modulations in the case of incommensurate structures), together with the atomic positions, is then restricted to an asymmetric unit under the relevant magnetic group. The magCIF format was rapidly implemented in most of the available computer tools for the analysis, visualization and determination of magnetic structures, allowing a direct communication among all these programs. In particular, during a visit in Bilbao, Robert M. Hanson, made the program Jmol fully compatible with magCIF files, both commensurate and incommensurate, and through his collaboration Jmol became the basic visualization tool of MAGNDATA. Also Koichi Momma kindly accepted our request and implemented the magCIF format in his program VESTA (for the moment only of commensurate structures), and VESTA came to be a very important help both for generating and checking new entries, and as an additional visualization tool in the database.

Since 2016, new entries are being steadily introduced. In June 2020 the collection had more than 1,000 magnetic structures, and by the time of this congress, it will have surpassed 2,000. Considering that the number of published magnetic structures with enough information may be several thousands and every year some hundred new ones are published, the database is still far from being complete, but its size is already very significant and allows massive searches and analyses (see for instance [3,4]). One must however emphasize that MAGNDATA does not make any validation check. Therefore the presence of a magnetic structure in the database is no guarantee of its correctness. In fact, it is not uncommon to find conflicting models of the same structure. In order to introduce a new structure the fundamental step is the construction of an appropriate magCIF file. This implies to interpret and translate the information of the original paper into the mentioned standardized description. In many cases this requires to identify for the first time the magnetic symmetry group of the proposed structure. This is usually done using the tools available in the magnetic section of the BCS or, specially in the case of incommensurate structures, in the ISOTROPY webpage [5]. Although the situation is improving, often the information provided in the article, specially in the case of incommensurate structures, is unfortunately incomplete or ambiguous, and these structures have been necessarily discarded.

In the long term MAGNDATA can only be kept updated, if the authors actively participate and directly submit their new published structures to the database in the form of magCIF files. This can be easily done following the instructions available in the webpage of the program. We hope that through the generalized use of this new direct submission option, MAGNDATA will consolidate as a freely available and very useful research tool in the field.