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The magneto-structural transformation materials, which experience the crystallographic and magnetic phase transition simultaneously, have attracted considerable attention not only for their importance in fundamental physics but also for their promising applications as multifunctional materials. Magnetic refrigeration based on the magnetocaloric effect (MCE) is a possible alternative to the current vapor compression technology [1]. Nowadays, most studies on magnetic refrigerants are focused on materials undergoing a first order phase transition because of their potential applications at room temperature.

The  $\text{CoMnGe}_{0.95}\text{Ga}_{0.05}$  compound was prepared by arc melting by using high-purity elements. Synchrotron experiments were performed in the temperature range between 290 and 390 K on B2 in HASYLAB/DESY in Hamburg. A synchrotron X-ray wavelength of 0.688105 Å was used. Magnetic measurements were performed as functions of temperature and magnetic fields with Physical Properties Measurements System-PPMS between 5 and 350 K under magnetic field up to 7 Tesla.

Synchrotron experiments shows that this compound exhibits the structural transition from high temperature phase (orthorhombic-space group: Pnma) to low temperature phase (cubic-space group:  $P6_3/mmc$ ) around the room temperature. According to Rietveld refinement, the unit cell volume of the high temperature phase is 77.3 Å<sup>3</sup> and the unit cell volume of low temperature phase is 160.9 Å<sup>3</sup> at 300 K.

According to temperature dependence of magnetization measurements, this compound has thermal hysteresis between FC and FH curves and this thermal hysteresis confirms the structural transition around  $T_C$ . While on FC mode the Curie temperature is 308 K, the Curie temperature is 319 K on FH mode. According to M(H) curves, this compound exhibit magnetic field induced structural transition. This magneto-structural transition makes this material very important for magnetic cooling technology. The magnetocaloric effect of this compound is estimated by using Maxwell equation. The magnetic entropy change is 4.5 J/kg.K and 30.9 J/kg.K for the magnetic field change of 1 Tesla and 7 Tesla, respectively.

This work was supported by The Scientific and Technological Research Council of Turkey-TÜBİTAK (Project Number: 109T743).

[1] V.K. Pecharsky, K.A. Gschneidner Jr., *Phys. Rev. Lett.* **1997**, 78, 4494.

**Keywords:** synchrotron experiments, magneto-structural transition, magnetic measurements

## MS96.P06

*Acta Cryst.* (2011) A67, C802

**Magnetic space groups: database and extinction rules for magnetic diffraction**

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Based on the recent compilations of magnetic space groups [1,2], a Magnetic Space Groups Database has been developed. This database is freely available on the Bilbao Crystallographic Server ([www.cryst.ehu.es](http://www.cryst.ehu.es)) [3], and includes useful data such as general positions (symmetry operations in matrix form), special Wyckoff positions, etc. Using this database and in order to facilitate the systematic use of extinction rules in magnetic non-polarized neutron diffraction analysis of magnetic structures, we have developed the computer tool MAGNEXT that is also freely available on the Bilbao Crystallographic Server. The

derivation of the extinction rules for magnetic diffraction is somewhat more complex compared with that of non-magnetic diffraction because of the axial vector character of the magnetic structure factor and its different and more complicated relation to the intensity. In fact, there are no listings of magnetic diffraction extinction rules comparable to those available for non-magnetic diffraction. This program is a contribution for changing this situation. MAGNEXT provides the extinction rules for non-polarized neutron diffraction corresponding to any Shubnikov magnetic space group. Illustrative examples are provided to demonstrate the utility of the program. Although not having the strong resolving power of the extinction rules of conventional non-magnetic crystallography, the extinction rules for magnetic diffraction can be useful for the systematic analysis and determination of magnetic structures, since they may facilitate the identification of their magnetic space group.

[1] H. Stokes, *Table of Magnetic Space Groups*: <http://stokes.byu.edu/magneticspacegroupshelp.html> [2] D. Litvin, *Acta Crystallographica* **2001**, A57, 729; *ibid* **2008**, A64, 419 (see also <http://www.bk.psu.edu/faculty/litvin/Download.html>) [3] M.I. Aroyo, J.M. Perez-Mato, C. Capillas, E. Kroumova, S. Ivantchev, G. Madariaga, A. Kirov, H. Wondratschek, *Zeitschrift fuer Kristallographie* **2006**, 221, 15.

**Keywords:** extinctions, magnetic symmetry, Bilbao crystallographic server

## MS96.P07

*Acta Cryst.* (2011) A67, C802-C803

**Magnetic structures of the family  $R_mM_n\text{In}_{3m+2n}$  of intermetallic compounds**

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The family  $R_mM_n\text{In}_{3m+2n}$  ( $R = \text{Ce} - \text{Tb}$ ;  $M = \text{Rh}, \text{Ir}$  or  $\text{Co}$ ;  $m = 1, 2$ ;  $n = 0, 1$ ) has been intensively investigated because its close relationship with the interesting physical properties found in other compounds of this family, specially for the  $R = \text{Ce}$  compounds, for whose a heavy fermion behavior with unconventional superconductivity (USC) has been reported. [1,2]

In this work we present a systematic study of the physical properties and the determination of magnetic structures of a new series of isostructural compounds  $R_mM_n\text{In}_{3m+2n}$  ( $R = \text{Gd}, \text{Tb}, \text{Sm}$ ;  $M = \text{Rh}, \text{Ir}$ ;  $m = 1, 2$ ;  $n = 0, 1$ ) exploring their relationship with physical properties of Ce-based compounds from this family. The magnetic structures of tetragonal  $\text{Gd}_2\text{IrIn}_8$ ,  $\text{GdRhIn}_5$ ,  $\text{TbRhIn}_5$ ,  $\text{Tb}_2\text{RhIn}_8$ ,  $\text{Sm}_2\text{IrIn}_8$  and cubic  $\text{GdIn}_3$  compounds have been determined using x-ray magnetic scattering (XRMS) at the bending magnet XRD2 beamline of the Laboratório Nacional de Luz Síncrotron (LNLS), in Campinas, Brazil. All these systems order antiferromagnetically in commensurate structures below their Néel temperatures ( $T_N$ ) with propagation vectors  $(1/2, 0, 0)$ ,  $(0, 1/2, 1/2)$ ,  $(1/2, 0, 1/2)$ ,  $(1/2, 1/2, 1/2)$ ,  $(1/2, 0, 0)$  and  $(1/2, 1/2, 0)$ , respectively [3-6]. The comparison between all the determined magnetic structures will be performed in terms of crystal field (CEF) effects along the series. The magnetic moments of rare earth ions are oriented in the tetragonal  $ab$ -plane for  $R = \text{Gd}$  and  $\text{Sm}_2\text{IrIn}_8$  compounds, while for the Tb-based systems order along the  $c$ -axis direction.  $T_N$  is increased along the tetragonal Tb-based compounds ( $\text{Tb1-1-5}$  and  $\text{Tb2-1-8}$ ) when compared to the cubic  $\text{TbIn}_3$  compound ( $T_N \sim 32$  K), as has been found for Nd-based compounds from this family [7].