



	Experiment title: Symmetry and structure of multiferroic Ba ₂ CoGe ₂ O ₇	Experiment number: 01-02-906 01-01-826
Beamline: BM01	Date of experiment: from: 16.09.2010 to: 21.09.2010	Date of report: 01.09.2013
Shifts: 9	Local contact(s): Dmitry Chernyshov, Wouter van Beek	<i>Received at ESRF:</i>

Names and affiliations of applicants (* indicates experimentalists):

V. Sikolenko¹, A. P. Sazonov^{2,3,*}, and V. Hutanu^{2,3,*}

¹Laboratory PSI WHGA/135, Paul Scherrer Institute, 5232 Villigen, Switzerland

²RWTH Aachen, Institut für Kristallographie, D-52056 Aachen, Germany

³Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at MLZ, D-85747 Garching, Germany

Report:

Coupled electric and magnetic orderings were recently found in Ba₂CoGe₂O₇ [1]. The symmetry information is essential to unravel the complex physics underlying magnetoelectric behavior of the title compound. Therefore, the crystal structure of Ba₂CoGe₂O₇ at room temperature (RT) and 90 K has been probed by single-crystal diffraction of x-ray synchrotron radiation. The space group (SG) found at both temperatures is well approximated by $P\bar{4}2_1m$, in agreement with expectation for melilite-like compounds. The real structure of Ba₂CoGe₂O₇ is more distorted and has a lower symmetry, as follows from observation of a set of superstructure reflections violating 2₁ symmetry. Symmetry analysis based on the observed average-structure SG $P\bar{4}2_1m$ revealed few possible candidates for the true structure that imposes different constraints on magnetic and polar properties.

TABLE I. The atomic position parameters of the average structure at RT ($P\bar{4}2_1m$).

Ion	Wyckoff Positions	x	Y	z
Ba	$4e$	0.33477(2)	0.16523(2)	0.49262(4)
Co	$2b$	0	0	0
Ge	$4e$	0.14051(3)	0.35949(3)	0.03963(7)
O1	$2c$	0	0.5	0.1588(8)
O2	$4e$	0.1384(2)	0.3616(2)	0.7284(5)
O3	$8f$	0.0799(2)	0.1843(2)	0.1876(3)

It is known that many of the melilite-like compounds show incommensurate or commensurate modulated lock-in phases at low temperatures [2]. A close inspection of our data for $\text{Ba}_2\text{CoGe}_2\text{O}_7$ revealed the following: (a) No incommensurate reections have been seen for the studied sample at both temperatures; (b) commensurate superstructure reections of type $(h, 0, 0)$, $(0, k, 0)$ with odd h and k , violating the systematic extinctions for the 2_1 symmetry element have been observed (Fig. 1). These reections are very weak yet observable up to $h, k = 13$ both at 90 K and RT. These observations allow us to conclude that the $P\bar{4}2_1m$ structure indeed is only an approximate one, and the true symmetry of $\text{Ba}_2\text{CoGe}_2\text{O}_7$ should be lower.

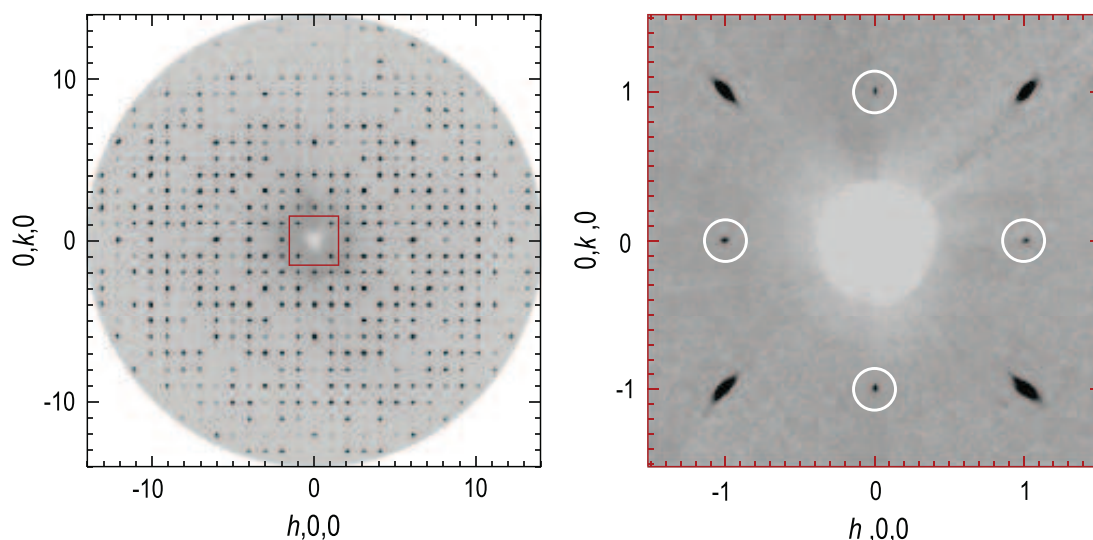


FIG. 1. (Color online) The $hk0$ layer calculated from two-dimensional detector images measured at 90 K; left: whole data set, right: magnified selected part with superstructure reflections noted by circles.

[1] H. T. Yi et al., Appl. Phys. Lett. 92, 212904 (2008).

[2] Z. H. Jia, Ph.D. thesis, University of Marburg, Germany, 2005.