ELSEVIER

Physica B 234–236 (1997) 569–571

PHYSICA B

Magnetic structure of Nd_2BaCoO_5

J. Hernández-Velasco[a,b,*], R. Sáez Puche[a], J. Rodríguez-Carvajal[b]

[a]*Dep. Química Inorgánica, Fac. CC. Químicas, U. Complutense, 28040-Madrid, Spain*
[b]*Lab. Léon Brillouin (CEA-CNRS), CE-Saclay, 91191 Gif sur Yvette Cedex, France*

Abstract

The magnetic behaviour of Nd_2BaCoO_5 has been studied by means of neutron powder diffraction at low temperatures. The magnetic structure is antiferromagnetic and can be described on the basis of a wave vector $\boldsymbol{k} = [\frac{1}{2}, 0, \frac{1}{2}]$ with a B_g magnetic mode, $T_N \sim 24$ K being the estimated Néel temperature. The Nd^{3+} magnetic moments are parallel to the crystallographic c-axis and the Co^{2+} magnetic moments lie in the ac plane oriented along the a-axis with a small canting in the z direction. Their values at 1.5 K are $2.55(4)\mu_B$ and $3.08(7)\mu_B$, respectively.

Keywords: Antiferromagnetism; Low-dimensional systems; Powder diffraction; Rietveld refinement

---

1. Introduction

R_2BaCoO_5 oxides (R = Rare Earth) form a large family of compounds with interesting magnetic properties and structural behaviour [1, 2]. For the biggest lanthanoid cations, like Nd, the crystal structure of these compounds belongs to the orthorhombic Immm space group and is characterized by the existence of one-dimensional arrangement of vertex connected (CoO_6) octahedra along the a-axis [1]. The oxides with the smallest rare earth ions present another type of structure belonging to the Pnma space group [2].

About the magnetic behaviour of the Immm-R_2BaCoO_5 oxides, one-dimensional correlations of antiferromagnetic character within the $(CoO_6)_n$ chains have been shown around RT [1], as it is inferred from the lack of the Co^{2+} magnetic moment contribution to the susceptibility. At lower temperatures, three-dimensional antiferromagnetic ordering has been proposed to explain the maximum observed in the susceptibility measurements, which in the case of the Nd_2BaCoO_5 takes place at 15 K [1].

The main purpose of this paper is to point out this assumption, solving for the first time the magnetic structure of this cobalt compound and comparing it with the isostructural R_2BaNiO_5 oxides, whose magnetic structures have been studied before [3, 4].

2. Experimental

Nd_2BaCoO_5 powder sample was prepared by a solid state reaction following the synthesis method described elsewhere [1]. The neutron diffraction data were obtained in the two axis diffractometer Pyrrhias at the Orphée reactor of the LLB, CEA-Saclay (France). The wavelength used was $\lambda = 2.426$ Å. The data were analyzed with the Rietveld method using the program FULLPROF [5].

---

* Corresponding author.

0921-4526/97/$17.00 © 1997 Elsevier Science B.V. All rights reserved
PII S0921-4526(96)01186-6

3. Results and discussion

The lattice parameters of Nd_2BaCoO_5 obtained at 1.5 K from the neutron diffraction data are the following: $a = 3.8095(3)$ Å, $b = 5.9441(5)$ Å and $c = 11.7690(9)$ Å.

From the evolution of the neutron diffraction patterns for the Nd_2BaCoO_5 oxide, the estimated Néel temperature is about $T_N \approx 24$ K. The magnetic reflections appearing below this temperature can be indexed in a commensurate lattice related to the crystallographic one by a propagation vector $k = [\frac{1}{2}, 0, \frac{1}{2}]$ [6]. The strongest coupling is the intrachain Co–Co, but it is worth noting that both the Nd^{3+} and Co^{2+} sublattices become ordered at the same temperature and so the intersite Nd–Co interaction is dominant over intrasite interactions of the type Nd–Nd or interchain Co–Co. It means that the coupling between the different magnetic atoms' sublattices requires that the basis vectors which describe the magnetic structure must belong to the same irreducible representation. In this way, using the representation analysis within the framework of group theory and following the method proposed by Bertaut [7], we have arrived at the different models of magnetic structures compatible with the crystal symmetry, which are summarized in Table 1, where the meaning of the $\boldsymbol{F}$ and $\boldsymbol{A}$ vectors is given by the linear spin combinations, $\boldsymbol{F} = \boldsymbol{m}_1 + \boldsymbol{m}_2$ and $\boldsymbol{A} = \boldsymbol{m}_1 - \boldsymbol{m}_2$, between the magnetic moment components of the two Nd sites 4*j*, i.e. $\pm(\frac{1}{2}\ 0\ z)$. While in the case of the Co sublattice, site 2*a* (0 0 0), the basis vectors are the spin components themselves.

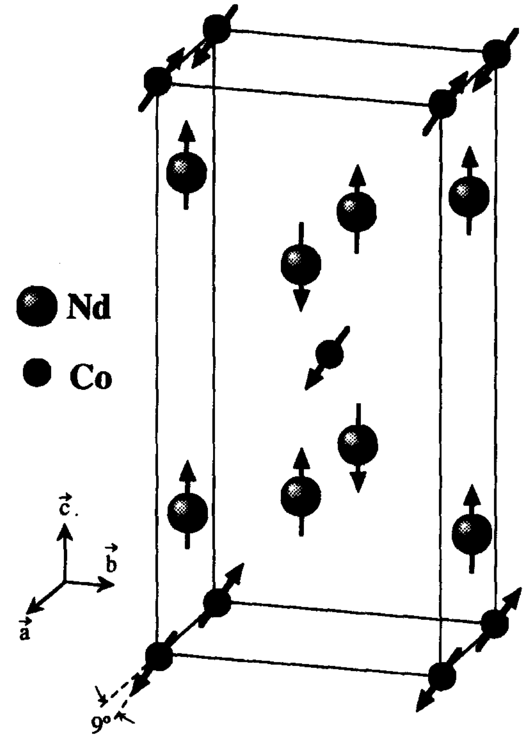

Fig. 1. Representation of the Nd_2BaCoO_5 magnetic structure at 1.5 K on one crystallographic cell excluding the non-magnetic atoms.

The fit of the experimental data agrees with a B_g symmetry representation, which means that the Co and Nd magnetic moments are restricted to the *ac* plane. The Nd magnetic moments $\boldsymbol{m}_{Nd}$ are parallel to the *c*-axis, as shown in Fig. 1, while $\boldsymbol{m}_{Co}$ are oriented antiferromagnetically along the *a*-axis with a small canting in the *z* direction ($m_z = 0.49(4)\mu_B$ and $m_x = -3.04(7)\mu_B$ at 1.5 K) and the order is ferromagnetic in the *b* direction. In this sense it is important to notice that both $\boldsymbol{m}_{Nd}$ and $\boldsymbol{m}_{Co}$ are nearly perpendicular, however in the case of the isostructural R_2BaNiO_5 oxides $\boldsymbol{m}_R$ and $\boldsymbol{m}_{Ni}$ are quite parallel, for example in the collinear structure proposed for Nd_2BaNiO_5 [3] or those canted but almost parallel spin models for R = Er or Ho [4]. This could be an indication of weakly coupled Nd^{3+} and Co^{2+} sublattices, only a very smooth Co^{2+} spin reorientation takes place while the ordered moment on the Nd site increases. The $\boldsymbol{m}_{Co}$ slightly rotate in the *ac* plane and change from pointing to the negative to point to the positive

Table 1
Basis vectors for Nd and Co sublattices

Γ	Nd			Co		
	x	*y*	*z*	*x*	*y*	*z*
A_g (+ +)	—	F	—	—	m	—
B_g (− +)	F	—	F	m	—	m
A_u (+ −)	A	—	A	—	—	—
B_u (− −)	—	A	—	—	—	—

direction of the c-axis between 16 and 14 K, which agrees with the temperature where a maximum appears in the magnetic susceptibility measurements [1].

When saturation is reached, the observed $\boldsymbol{m}_{\mathrm{Nd}} = 2.55(4)\mu_{\mathrm{B}}$ value is lower than $gJ = 3.27\mu_{\mathrm{B}}$, which can be due to the splitting of the ground state level by the crystal field, similar effects have been observed in the $\boldsymbol{m}_{\mathrm{R}}$ on the isostructural $\mathrm{R_2BaNiO_5}$ [3, 4]. The $\boldsymbol{m}_{\mathrm{Co}} = 3.08(7)\mu_{\mathrm{B}}$ experimental value at 1.5 K is near $2S = 3\mu_{\mathrm{B}}$ but slightly higher, as we have observed, even more marked, in other Immm and Pnma $\mathrm{R_2BaCoO_5}$ oxides. This really shows that opposite effects are cancelled which are on the one hand the strong orbital angular contribution to the moment which increases its value, and on the other hand the covalency and low dimensional effects (quantum spin fluctuations) which tend to decrease the magnetic moment value from the expected one. The latter effect is observed in the Ni compounds [3, 4], where L does not have an important role.

References

[1] J. Hernández-Velasco, A. Salinas and R. Sáez-Puche, J. Solid State Chem. 110 (1994) 321.
[2] J. Hernández-Velasco, A. Salinas, F. Fernández and R. Sáez-Puche, J. Alloys Comp. 203 (1994) 15.
[3] V. Sachan, D.J. Buttrey, J.M. Tranquada and G. Shirane, Phys. Rev. B 49 (1994) 9658.
[4] E. García-Matres, J. Rodríguez-Carvajal, J.L. Martínez, A. Salinas and R. Sáez-Puche, Solid State Commun. 85 (1993) 553.
[5] J. Rodriguez-Carvajal, Physica B 192 (1993) 55.
[6] J. Hernández-Velasco, R. Sáez-Puche, J. Rodríguez-Carvajal, E. García-Matres and J.L. Martínez, J. Alloys Compounds 207/208 (1994) 257.
[7] E.F. Bertaut, Acta Crystallogr. A 24 (1968) 217.