Evidence of low-dimensional antiferromagnetic ordering and crystal structure in the R_2BaNiO_5 (R = Y,Er) oxides

J. Amador, E. Gutiérrez-Puebla,* M. A. Monge,* I. Rasines,† and C. Ruíz-Valero*
Instituto de Ciencia de Materiales, Consejo Superior de Investigaciones Científicas, Serrano 113, 28006 Madrid, Spain

F. Fernández and R. Sáez-Puche
Departamento de Química Inorgánica, Facultad de Ciencias Químicas, Universidad Complutense, 28040 Madrid, Spain

J. A. Campá
Departamento de Cristalografía y Mineralogía, Facultad de Ciencias Geológicas, Universidad Complutense, 28040 Madrid, Spain

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Crystals of R_2BaNiO_5 (R=Y,Er) have been grown, and their structures have been established by single-crystal x-ray diffraction. Both compounds crystallize in the Nd_2BaNiO_5 structure type, with one-dimensional chains of vertex-sharing NiO_6 octahedra in the direction of the **a** axis. These octahedra show an unusual twofold distortion: The Ni-O distances to the two axial oxygen atoms are considerably shorter, 0.3 Å, than those to the four equatorial oxygens, and these oxygens are distorted from the right angles of a regular octahedron to 79.0(2)° or 77.7(6)°, respectively. As a result of this, Ni-O(axial)-Ni distances are very short, 3.76 and 3.75 Å for R=Y and Er, respectively. X-ray powder diffraction data and the results of magnetic measurements for both oxides are given. The structural features mentioned elucidate why Ni^{2+} ions in polycrystalline Y_2BaNiO_5 behave as a monodimensional system in which they become antiferromagnetically ordered below 300 K. Besides that, the ferromagnetic interactions that operate below 40 K can be due to tridimensional interchain interactions and/or the presence of ferromagnetic impurities. The estimated Néel temperature for Y_2BaNiO_5, higher than that reported for Y_2BaCuO_5, is explained by the promotion of the superexchange Ni-O-Ni interactions along the chains of flattened NiO_6 octahedra sharing corners. In Er_2BaNiO_5 both effects are masked by the strong paramagnetic signal of Er^{3+}, and a maximum observed at 15.6 K for the susceptibility is attributed to tridimensional ordering of the Er^{3+} cations.

INTRODUCTION

Polycrystalline samples of a new family of oxides of general formula R_2BaMO_5, where R stands for a trivalent rare-earth cation and M represents Cu or Zn, were first prepared and characterized by the group of Raveau[1,2] in the early 1980s. The Cu compounds with R from Sm to Tm are isostructural,[1] space group (SG) *Pnma*, and have a framework built up through edge and face sharing of RO_7 monocapped trigonal prisms, with the M atoms showing a pyramidal MO_5 coordination, which has been established[3,4] in single crystals of two compounds. The R_2BaCuO_5 oxides, which appear sometimes as impurities of the new high-temperature superconductors of the composition $RBa_2Cu_3O_{7-x}$, have been designed as the *green phases,* while the isostoichiometric Zn compounds, being light colored, have been studied from the point of view of their optical properties.[5] As for Y_2BaCuO_5, magnetic measurements and neutron diffraction studies have shown[6] that copper moments order antiferromagnetically in this oxide at about 28 K.

The first example of a new family of oxides formulated as R_2BaNiO_5 (R=Nd) was described by Müller-Buschbaum and co-workers[7] in the SG *Immm*. Unlike tetragonal pyramidal Cu or Zn in R_2BaMO_5, Ni in Nd_2BaNiO_5 forms chains of flattened NiO_6 octahedra with four oxygens at a larger distance than the other two. Subsequent studies established[8–10] the same crystal structure for the majority of the compounds with R from Sm to Tm. Independently, our group prepared and characterized[11] polycrystalline samples of nine R_2BaNiO_5 oxides (R=Y, Nd, Sm, Eu, Gd, Dy, Ho, Er, or Tm) and, after growing single crystals, determined[12] the structure of the Gd compound following an anisotropic refinement which led to a discrepancy factor of 0.019 and to the following Ni-O internuclear distances: 4 of 2.197(6) Å and 2 of 1.8936(2) Å. This unusual distortion away from the ordinary octahedral coordination about Ni, as well as the existence of one-dimensional (1D) chains of vertex-sharing octahedra in the direction of the **a** axis with extremely short Ni-O-Ni distances (3.79 Å in the Gd compound[12]), suggested interesting physical properties.

On the other hand, nearest oxygens to Ni are distorted from the 90° angles of a regular octahedron to 79.6(2)°. These observations[12] have been recently shown[13] understandable using a model which combines results from

molecular-orbital theory, tight-binding band-structure calculations, and empirical atom-atom potential arguments. In order to apply this combination of methods, x-ray diffraction data are needed from anisotropic refinements as good as possible. In addition, the possibility of obtaining nonstoichiometric samples of these oxides cannot be conclusively discarded: For example, in the case of the Cu compounds, it seems that nonstoichiometric crystals have been obtained.[4] In these cases precise x-ray diffraction data are also needed for determining the population factors of the oxygen atoms. In the present paper we report the interesting magnetic properties of two of these oxides, R_2BaNiO_5 (R=Y,Er), as well as their crystal structures and x-ray diffraction data. As far as we know, one of them, R=Y, has been prepared for the first time. Although the crystal structure of the Er compound is known,[8] it was determined through an isotropic refinement which led to a high discrepancy factor, 0.103.

EXPERIMENTAL ASPECTS

Tiny prismatic crystals, black colored, of composition R_2BaNiO_6 (R=Y,Er) were grown after adding R_2O_3 to a mixture of an excess of Ni metal with $Ba(OH)_2\cdot 8H_2O$ held at 100 °C, heating to 1150 °C, and quenching in air. Er_2BaNiO_5 crystals were polysynthetically twinned. The crystals were mounted in a Kappa diffractometer. A summary of the fundamental crystal and refinement data is given in Table I. The cell dimensions were refined by least-squares fitting the 2θ values of 25 reflections. The intensities were corrected for Lorentz and polarization effects. Scattering factors for neutral atoms and anomalous dispersion corrections for Y, Er, Ba, and Ni were taken from the International Tables for X-ray Crystallography.[14] The structure was solved by Patterson and Fourier methods. An empirical absorption correction was applied at the end of the isotropic refinement.[15] After anistropic full-matrix least-squares refinement, a final difference synthesis had no significant electron density. Most of the calculations were carried out with the X-ray 80 System.[16] Polycrystalline R_2BaNiO_5 (R=Y,Er) samples for magnetic measurements were prepared from stoichiometric mixtures of analytical grade R_2O_3, BaO_2, and NiO, that were ground, pelletized, and heated in air for 12 h at 900, 1000, 1100, and 1200 °C. After each thermal treatment, the products were quenched, reground, and pelletized. The x-ray diffraction data for polycrystalline samples were measured and calculated as indicated elsewhere.[17] For the calculation of the intensities of polycrystalline R_2BaNiO_5 (R=Y,Er) the atomic positions and temperature factors obtained after solving the crystal structures were employed. Magnetic susceptibility measurements were made in the 4.2–300 K temperature range as pointed out elsewhere.[17] The susceptibility, χ, was independent of the field at all temperatures for Er_2BaNiO_5, while in the case of the Y compound a small susceptibility dependence with the temperature below 40 K was observed. The molar susceptibilities were corrected for ionic diamagnetism using the values,[18] in 10^{-6} emu mol^{-1}, of -12 for O^{2-}, Ni^{2+} and Y^{3+}; -18 for Er^{3+}; and -32 for Ba^{2+}.

TABLE I. Crystal and refinement data for R_2BaNiO_5 (R=Er,Y).

Formula	$BaEr_2NiO_5$	BaY_2NiO_5
Crystal system	Orthorhombic	Orthorhombic
Space group[a]	*Immm*	*Immm*
a (Å)	3.747(2)	3.7610(6)
b (Å)	5.737(2)	5.7610(7)
c (Å)	11.283(2)	11.323(2)
V (Å^3)	242.5(2)	245.34(7)
Z	2	2
F(000)	520	404
ρ (calc) (g cm^{-3})	8.36	6.14
t (°C)	21	21
μ (cm^{-1})	465.2	352.3
Cryst. dimens. (mm^3)	0.1×0.1×0.25	0.04×0.04×0.2
Diffractomer	Enraf-Nonius CAD4	Enraf-Nonius CAD4
Radiation	Graphite-monochromated Mo $K\alpha$ (λ=0.710 69 Å)	Graphite-monochromated Mo $K\alpha$ (λ=0.710 69 Å)
Scan technique	$\Omega/2\theta$	$\Omega/2\theta$
Data collected	(0,0,0) to (5,8,16)	(0,0,0) to (5,8,16)
Unique data	250	254
Unique data (I)$\geq 2\sigma(I$)	249	228
Std. rflns.	3 rflns.	3 rflns.
Decay	≤1% variation	
R_F[b] (%)	4.4	2.3
Average shift/error	0.006	0.002
Maximum shift/error	0.03	0.01

[a]Reference 14, Vol. IV, pp. 314–315.
[b]$R_F=\sum_{\text{refl}}(|F_{\text{obs}}|-|F_{\text{calc}}|)/\sum_{\text{refl.}}|F_{\text{obs}}|$.

TABLE II. Atomic coordinates and isotropic temperature factors for R_2BaNiO_5, with standard deviations in parentheses.

Atom	*x*/*a*	*y*/*b*	*z*/*c*	U_{eq} [a]
Y	0	0	0.2027(1)	1.8(3)
Ba	0	0.5	0	5.1(3)
Ni	0.5	0	0	2.7(5)
O(1)	0.5	0.2408(8)	0.1487(3)	5(1)
O(2)	0	0	0	4(2)
Er	0	0	0.2031(1)	3(1)
Ba	0	0.5	0	7(1)
Ni	0.5	0	0	6(1)
O(1)	0.5	0.2385(29)	0.1507(13)	14(4)
O(2)	0	0	0	13(9)

[a] $U_{eq}=\frac{1}{3}\sum_{i,j}[U_{ij}a_i^*a_j^*a_ia_j\cos(a_i,a_j)]\times 10^{-3}$.

RESULTS AND DISCUSSION

Crystal structure

Atomic coordinates for R_2BaNiO_5 (R=Y,Er) are shown in Table II. Table III includes bond lengths and angles. For R=Er all the dimensions are very similar to those of the Y compound. There are three slightly different R-O distances, as Table III shows. RO_7 polyhedra share different elements in each direction of the space giving rise to two kinds of interstices. Those in the **a** direction (Fig. 1) show the form of flattened octahedra with four equal NiO(1) equatorial distances and two NiO(2) apical, 0.3 Å shorter. The NiO_6 flattened octahedra share O(2) vertices with each other, being the Ni-O-Ni distances 3.76 and 3.75 Å, respectively, even shorter than in the Gd compound.[12] The interstices formed in the **b** direction are bicapped quadrangular cavities which house the Ba^{2+} cations. These three kinds of polyhedra converge at the O(2) atoms, and the structure consists of blocks of RO_7 polyhedra sharing two edges of their largest quandrangular faces, in the **a** direction. Two of these blocks are opposite each other in the **c** direction, as Fig. 2 shows, and share the vertex occupied by the O(2) atom. The set formed by two blocks is joined along the **b** direction to the other two sets, one placed above it and the other below. This second set is also shown in Fig. 2.

TABLE III. Bond distances (Å) and angles (°) and principal interatomic distances in BaR_2NiO_5.

			R=Er	R=Y
Ba	O(1)	[8]	2.941(12)	2.933(3)
	O(2)	[2]	2.869(1)	2.8805(3)
R	O(1)	[4]	2.394(10)	2.416(3)
	O(1)	[2]	2.229(15)	2.250(4)
	O(2)	[1]	2.292(1)	2.2952(8)
Ni	O(1)	[4]	2.183(15)	2.182(4)
	O(2)	[2]	1.874(1)	1.8805(3)
R	*R*	[4]	3.586(1)	3.6029(4)
		[2]	3.747(2)	3.7610(6)
Ni	Ni	[2]	3.747(2)	3.7610(6)
O(1)-Ni-O(1)		[2]	180.0(3)	180.0(5)
		[2]	102.3(6)	101.0(2)
		[2]	77.7(6)	79.0(2)
O(1)-Ni-O(2)		[8]	90.000(1)	90.000(2)
O(2)-Ni-O(2)		[1]	180	180

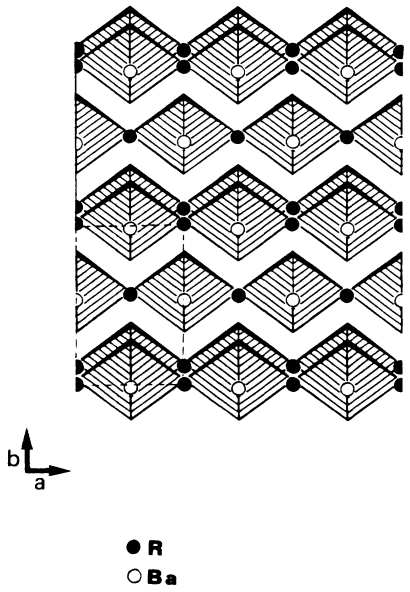

FIG. 1. View along the **c** direction (rotated 10°) showing the chains of NiO_6 octahedra.

Magnetic measurements

Tables IV and V show the x-ray diffraction data for polycrystalline samples of the Y and Er compounds, re-

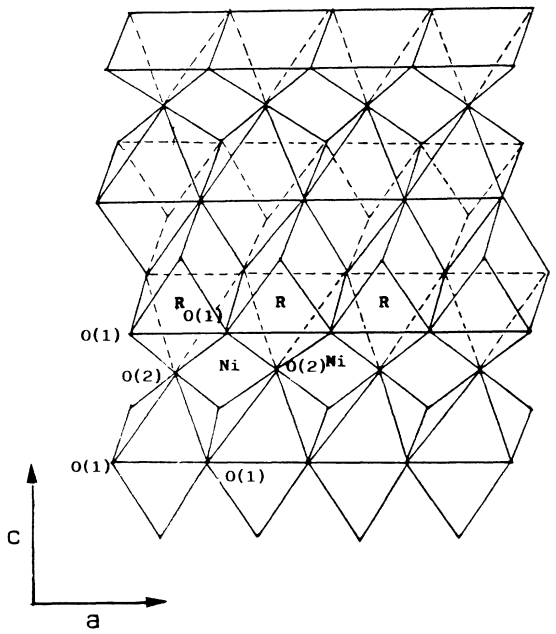

FIG. 2. Perspective of the packing of RO_7 polyhedra in the crystal structure of R_2BaNiO_5.

spectively. The temperature dependence of the magnetic susceptibility for Y_2BaNiO_5 is shown in Fig. 3. A progressive decreasing in the susceptibility can be observed with decreasing temperatures until 60 K. Below this temperature the susceptibility remains almost constant until 20 K. At the lowest temperatures down to 4.2 K a sharp field dependence increasing is observed. The susceptibility at room temperature is 1.093×10^{-3} emu mol^{-1}, a value rather smaller than that expected for Ni^{2+} with two unpaired localized electrons and $S=1$. This behavior can be attributed to the superexchange interactions due to the strong O-e_g-O overlapping at 180° of the oxygen p orbitals and the Ni^{2+} d orbitals giving rise to strong antiferromagnetic interactions. These interactions are more intense than those present in La_2NiO_4, although Ni^{2+} ions have two magnetic neighbors in linear Y_2BaNiO_5 and four in layered La_2NiO_4. The shorter Ni-O-Ni distances in Y_2BaNiO_5, 3.76 Å, as compared with those[19] in La_2NiO_4, 3.86 Å, justify for the Y oxide a more effective O-e_g-O overlapping, stronger superexchange interactions, and the ordering of the Ni^{2+} ions along the chains of NiO_6 flattened octahedra at room temperature. The increase of susceptibility observed below 20 K could be due to two possible causes. At these low temperatures

TABLE IV. X-ray diffraction data for polycrystalline Y_2BaNiO_5.

h	k	l	d_{obs}	d_{calc}		I_{obs}	I_{calc}	h	k	l	d_{obs}	d_{calc}		I_{obs}	I_{calc}
0	0	2	5.68	5.67		18	22	3	2	1	1.1434	1.1434	>	43	16
0	1	1	5.15	5.14		13	8	2	4	0		1.1433	>		46
1	0	1	3.572	3.568		93	98	0	0	10	1.1332	1.1332		12	14
0	1	3	3.160	3.159		277	283	1	2	9		1.1029	>		12
0	2	0	2.881	2.880		279	279	0	5	3	1.1018	1.1021	>	19	12
0	0	4	2.834	2.833		113	122	3	0	5	1.0969	1.0968		18	18
1	1	2	2.753	2.752		1000	1000	1	3	8	1.0909	1.0909		32	41
1	0	3	2.653	2.665		12	2	1	5	2	1.0814	1.0814		39	46
0	2	2	2.5686	2.5677		25	22	2	4	4	1.0603	1.0602		19	21
1	2	1		2.2415			175	0	2	10	1.0546	1.0545		31	36
0	1	5		2.1090	>		34	2	3	7	1.0338	1.0338		24	24
1	1	4	2.1072	2.1060	>	72	45	3	3	2	1.0320	1.0320		35	42
0	2	4	2.0198	2.0198		189	199	3	1	6	1.0280	1.0276		12	7
1	2	3	1.9564	1.9561		45	42	3	2	5	1.0249	1.0250		24	29
1	0	5	1.9416	1.9411		126	128	2	4	6	0.9783	0.9781		19	24
0	0	6	1.8891	1.8886		66	61	2	0	10	0.9706	0.9705		15	20
2	0	0	1.8804	1.8801		141	148	0	6	0	0.9600	0.9602		12	10
0	3	3	1.7118	1.7118		43	41	2	5	3	0.9507	0.9508		15	20
1	3	2	1.6371	1.6372		180	198	4	0	0	0.9400	0.9400		15	15
1	1	6	1.6199	1.6196		42	34	0	5	7	0.9389	0.9387		16	10
2	1	3	1.6156	1.6156		93	77	1	6	1		0.9271			11
1	2	5	1.6097	1.6097		137	124	3	1	8	0.9266	0.9264		27	33
0	2	6		1.5794			32	2	2	10	0.9196	0.9197		42	60
2	2	0	1.5749	1.5744		96	86	1	4	9		0.9192			14
2	0	4	1.5667	1.5665		46	39	0	6	4		0.9094			15
0	1	7	1.5584	1.5585		40	38	1	1	12	0.9046	0.9045		28	41
1	0	7	1.4882	1.4869		13	10	4	1	3	0.9011	0.9010		17	18
0	3	5		1.4651	>		9	4	2	0	0.8937	0.8937		17	20
1	3	4	1.4644	1.4641	>	22	16	0	4	10	0.8906	0.8906		17	20
0	4	0	1.4409	1.4402		56	54	3	4	5	0.8725	0.8726		19	31
2	1	5	1.4037	1.4034		18	15	1	5	8	0.8696	0.8696		23	36
2	2	4	1.3760	1.3762		73	94	1	6	5	0.8605	0.8606		19	31
1	4	1	1.3355	1.3359		16	12	4	1	5	0.8586	0.8586		14	5
2	0	6	1.3325	1.3324		35	32	2	6	0		0.8551			23
1	1	8		1.2918			73	4	2	4	0.8523	0.8523		21	34
0	4	4	1.2839	1.2839		24	19	3	2	9		0.8488			12
2	3	3	1.2657	1.2657		26	30	3	3	8	0.8435	0.8433			38
0	3	7	1.2377	1.2377		16	19	2	5	7	0.8394	0.8398		23	23
2	2	6	1.2093	1.2093		14	24	3	5	2	0.8390	0.8388		25	44
2	1	7	1.1998	1.1998		30	31	1	3	12	0.8266	0.8267		23	53
3	1	2	1.1971	1.1971		59	63	4	3	3		0.8240			23
1	0	9		1.1939			12	2	6	4	0.8186	0.8186		16	40
1	4	5	1.1565	1.1566		37	42	4	1	7		0.8049			34
0	4	6	1.1452	1.1452		21	18	2	4	10	0.8049	0.8048		34	62
								1	7	2	0.7959	0.7960		25	69

it is possible that some interchain ferromagnetic interactions could be operative, giving rise to a tridimensional magnetic order; however, the presence and/or some ferromagnetic impurities cannot be discarded.

The reciprocal susceptibility for Er_2BaNiO_5 is displayed in Fig. 4. In the 300–40 K temperature range a Curie-Weiss behavior can be observed, since $\chi = 11.50/(T+0.94)$. Below 40 K the experimental data exhibit a strong deviation from the Curie-Weiss law and the curve bends upward showing a minimum at 15 K. The magnetic moment calculated from the Curie-Weiss law is $9.59\mu_B$ which fairly agrees with that expected, $9.6\mu_B$, for the free Er^{3+} ion.[20] The contribution to the susceptibility of Ni^{2+}, expected to be antiferromagnetically ordered as in isostructural Y_2BaNiO_5, should be very small and will be masked by the strong paramagnetic signal due to the f electrons of the Er^{3+} ions. The low-temperature data are better illustrated in the χ versus T plot, as shown in the inset in Fig. 4. The maximum observed in χ at 15.6 K can be attributed to tridimensional antiferromagnetic ordering of the Er^{3+} ions. Below this temperature the susceptibility sharply falls in such a way that the magnetic moment of Er^{3+} at the liquid helium temperature only reaches about $3\mu_B$. This is unusual and

TABLE V. X-ray diffraction data for polycrystalline Er_2BaNiO_5.

h	k	l	d_{obs}	d_{calc}		I_{obs}	I_{calc}	h	k	l	d_{obs}	d_{calc}		I_{obs}	I_{calc}
0	0	2	5.68	5.65		19	20	3	2	1		1.1406			14
0	1	1	5.19	5.11		19	20	2	4	0	1.1399	1.1393		47	44
1	0	1	3.571	3.561		103	102	0	0	10	1.1292	1.1293		13	15
0	1	3	3.177	3.147		356	344	1	2	9		1.0991	>		13
0	2	0	2.874	2.868		304	304	0	5	3	1.0977	1.0974	>	22	14
0	0	4	2.829	2.823		123	105	3	0	5	1.0945	1.0942		26	22
1	1	2	2.749	2.744		1000	1000	1	3	8	1.0870	1.0870		32	40
1	0	3	2.663	2.658		19	14	1	5	2	1.0772	1.0769		38	46
1	2	1		2.2336			148	2	4	4	1.0565	1.0562		14	18
0	1	5	2.1028	2.1016		80	72	0	2	10	1.0508	1.0508		26	35
1	1	4		2.0995			10	1	4	7		1.0306	>		10
0	2	4	2.0115	2.0120		162	155	2	3	7	1.0304	1.0303	>	36	28
1	2	3	1.9512	1.9493		85	80	3	3	2	1.0295	1.0292		40	42
1	0	5	1.9362	1.9351		157	153	3	2	5	1.0224	1.0223		29	35
0	0	6	1.8828	1.8822		62	44	2	4	6	0.9749	0.9747		15	18
2	0	0	1.8775	1.8761		140	141	2	0	10	0.9678	0.9676		16	21
0	3	3	1.7050	1.7047	>	65	52	0	6	0	0.9564	0.9560		9	11
1	3	0		1.7036	>		11	2	5	3	0.9477	0.9473		17	22
1	3	2	1.6315	1.6310		188	198	4	0	0		0.9381	>		15
1	1	6		1.6144			15	0	5	7	0.9352	0.9349	>	20	12
2	1	3	1.6115	1.6115		96	94	3	1	8	0.9240	0.9239		30	32
1	2	5	1.6047	1.6041		161	151	1	6	1		0.9233			10
0	2	6		1.5736			24	2	2	10	0.9168	0.9168		47	58
2	2	0	1.5709	1.5701		92	95	1	4	9		0.9158			14
2	0	4	1.5633	1.5626			34	0	6	4	0.9059	0.9055		11	12
0	1	7	1.5531	1.5531		52	48	1	1	12	0.9014	0.9015	>	59	43
1	0	7	1.4822	1.4821		20	19	4	1	3	0.8992	0.8990	>		22
0	3	5	1.4596	1.4593		22	20	4	2	0	0.8919	0.8916		16	22
0	4	0	1.4348	1.4340		51	52	0	4	10	0.8875	0.8872		18	22
2	1	5	1.3998	1.3996		35	33	3	4	5	0.8699	0.8701		18	37
2	2	4	1.3723	1.3721		61	74	1	5	8	0.8667	0.8662		23	35
1	4	1	1.3310	1.3302		19	12	1	6	5	0.8574	0.8571		26	37
2	0	6	1.3289	1.3287		29	23	4	1	5		0.8566			11
1	1	8	1.2877	1.2875			71	2	6	0	0.8525	0.8518		18	24
0	4	4	1.2791	1.2785		17	17	4	2	4	0.8503	0.8502		25	27
2	3	3	1.2617	1.2620		39	34	3	2	9		0.8464			12
0	3	7	1.2333	1.2330		19	23	3	3	8	0.8410	0.8408		25	37
3	1	0	1.2100	1.2220		8	3	2	5	7	0.8368	0.8368		31	30
2	2	6	1.2059	1.2057		22	19	3	5	2		0.8361			45
2	1	7	1.1965	1.1964		44	40	1	3	12	0.8238	0.8238		30	55
3	1	2	1.1946	1.1944		57	63	2	6	4	0.8158	0.8155		18	33
1	0	9		1.1900			11	4	1	7		0.8029			41
1	4	5	1.1524	1.1521	>	54	50	2	4	10	0.8022	0.8021		32	69
2	3	5		1.1519	>		15	1	7	2	0.7929	0.7926		27	73
0	4	6		1.1407			13								

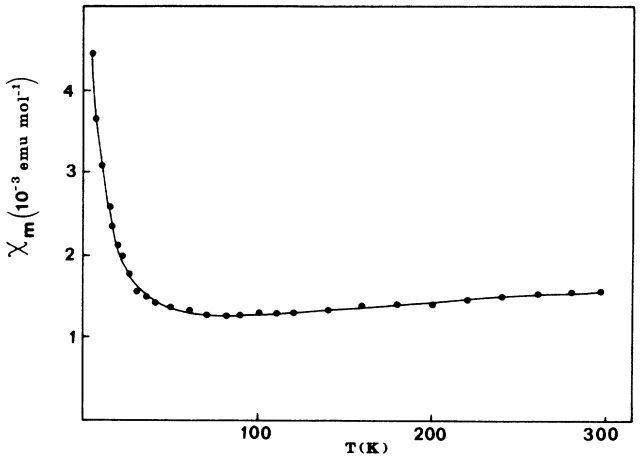

FIG. 3. Temperature dependence of the magnetic susceptibility per mole of Ni^{2+} of Y_2BaNiO_5.

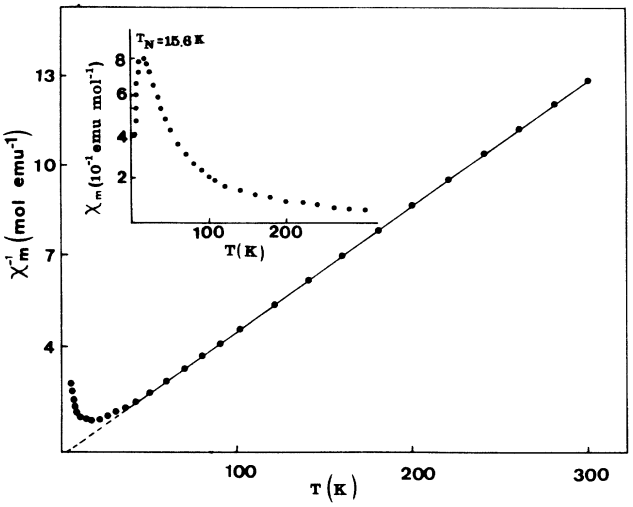

FIG. 4. Temperature variation of the reciprocal magnetic susceptibility per mole of Er^{3+} in Er_2BaNiO_5. In the inset, plotting of the magnetic susceptibility per mole of Er^{3+} in Er_2BaNiO_5, as a function of the temperature.

indicates strong interactions which mask the expected crystal-field effect ordinarily present in the Er mixed oxides at this lower temperature.[21,22] Although antiferromagnetic order has been recently reported in some R_2MO_4 oxides, R being a rare earth and M equal to Ni or Cu, in all cases the Néel temperatures are[23,24] below 15.6 K.

In summary, the oxides formulated R_2BaNiO_5 (R=Y,Er) exhibit very interesting structural and magnetic properties. In the Y compound, chains of NiO_6 flattened octahedra and extremely short Ni-O-Ni distances explain the behavior of Ni^{2+} ions as a monodimensional 1D system, in which they become antiferromagnetically ordered below 300 K. Moreover, in the Y oxide some ferromagnetic interactions are operative below 40 K as a consequence of tridimensional interchain interactions and/or the presence of ferromagnetic impurities. The estimated Néel temperature for this oxide is comparatively higher than the value of 28 K reported[6] from neutron diffraction data for the analogous Y_2BaCuO_5. The mentioned structural differences between both compounds should be responsible for such distinct behavior. Whereas in Y_2BaNiO_5 the superexchange Ni-O-Ni is clearly promoted along the chains of sharing-corners flattened NiO_6 octahedra, the low Néel temperature of 28 K for Y_2BaCuO_5 is due to the absence of a direct network Cu-O-Cu superexchange path in its structure. In the case of the Er oxide, both effects are masked by the strong paramagnetic signal of Er^{3+}, and the maximum observed for the susceptibility at 15.6 K can be attributed to a tridimensional ordering of the Er^{3+} ions.

Although the key factor of the interesting properties exhibited by the R_2BaNiO_5 oxides appears to be the presence of chains of flattened NiO_6 octahedra with short Ni-O-Ni distances, we have grown crystals of the Nd, Sm, Eu, Dy, and Ho compounds and we are performing magnetic measurements on polycrystalline samples of these oxides to further elucidate the nature of the antiferromagnetic order which they exhibit. We are also currently undertaking neutron diffraction measurements to explore their magnetic structure. Listings of anisotropic thermal parameters for Y_2BaNiO_5 are Er_2BaNiO_5 and of observed and calculated structure factors are available.[25]

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*Also at the Grupo de Difracción; Facultad de Ciencias Quimicas, Universidad Complutense, 28040 Madrid, Spain.
†Author to whom correspondence should be addressed.

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[25]See AIP document No. PAPS-PRBMD-42-7918-06 for listings of anisotropic thermal parameters for Y_2BaNiO_5 (1 page) and Er_2BaNiO_5 (1 page); and listings of observed and calculated structure factors for Y_2BaNiO_5 (2 pages) and Er_2BaNiO_5 (2 pages). Order by PAPS number and journal reference from American Institute of Physics, Auxiliary Publication Service, 335 East 45th Street, New York, NY 10017. The prices are $1.50 for microfiche and $5 for photocopies. Airmail additional. Make checks payable to the American Institute of Physics.