Magnetic structure of $Er_2Cu_2O_5$

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According to neutron-diffraction data at 1.9 K, the magnetic moments of copper [$1.0(1)\mu_B$] are directed along the **b** axis and form ferromagnetic layers of alternating sign parallel to the **ab** plane. The magnetic moments of Er1 [$5.36(5)\mu_B$] and Er2 [$3.96(7)\mu_B$] lie in the **bc** plane.

A pronounced diversity of magnetic properties is observed[1] in the series of isomorphous compounds $R_2Cu_2O_5$ (R = Tb–Lu), evidently because of a significant polarization of the rare earth. In a previous study[2] we reported on the ordering of the Cu^{2+} spins in the absence of a magnetic rare-earth subsystem ($Lu_2Cu_2O_5$). In the present letter we report the magnetic structure found for $Er_2Cu_2O_5$ by neutron diffraction.

A polycrystalline sample of a single phase was synthesized by the procedure of Ref. 1. Since two peaks were observed in the magnetic susceptibility ($T_N = 24$ K and $T_1 = 12$ K) in Ref. 1, we recorded three neutron diffraction patterns, at temperatures of 30 K, 16 K, and 1.9 K. These measurements were carried out on a diffractometer with the position-sensitive detector of the SILOÉ reactor.

The systematic classification of the magnetic reflections at each of the two temperatures below T_N indicates that the wave vector of the magnetic structure is $\mathbf{k} = 0$. The basis functions of the four irreducible representations of the group of this wave vector are

$$\Gamma_1(G_i^x, A_i^y, C_i^z;\ g_i^x, a_i^y, c_i^z),$$
$$\Gamma_2(A_i^x, G_i^y, F_i^z, a_i^x, g_i^y, f_i^z),$$
$$\Gamma_3(F_i^x, C_i^y, A_i^z, f_i^x, c_i^y, a_i^z),$$
$$\Gamma_4(C_i^x, F_i^y, G_i^z, c_i^x, f_i^y, g_i^z),$$

where

$$\mathbf{F}_i = \frac{1}{2}(\mathbf{S}_{i1} + \mathbf{S}_{i2} + \mathbf{S}_{i3} + \mathbf{S}_{i4}),$$
$$\mathbf{C}_i = \frac{1}{2}(\mathbf{S}_{i1} + \mathbf{S}_{i2} - \mathbf{S}_{i3} - \mathbf{S}_{i4}),$$
$$\mathbf{G}_i = \frac{1}{2}(\mathbf{S}_{i1} - \mathbf{S}_{i2} + \mathbf{S}_{i3} - \mathbf{S}_{i4}),$$
$$\mathbf{A}_i = \frac{1}{2}(\mathbf{S}_{i1} - \mathbf{S}_{i2} - \mathbf{S}_{i3} + \mathbf{S}_{i4})$$

TABLE I.

T, K / hkl	T = 1,9 K		T = 16 K	
	I_{obs}	I_{calc}	I_{obs}	I_{calc}
001	173 (2)	172	75 (2)	67
100	52 (2)	55	38 (2)	38
101	66 (2)	68	34 (2)	35
200 + 102	107 (3)	98	56 (2)	56
201	333 (3)	324	188 (3)	184
003	205 (3)	214	122 (3)	123
202	26 (2)	20	14 (2)	10
103	1 (2)	1	3 (2)	6
300	16 (2)	21	14 (2)	11
020 + 301	11 (2)	8	4 (2)	5
R %	5.1		4.6	

for the copper moments $\mathbf{S}_{ij}$; $\mathbf{f}_i$, $\mathbf{c}_i$, $\mathbf{g}_i$, $\mathbf{a}_i$ are the corresponding combinations of the erbium moments $\mathbf{S}_{ij}$. The index $i = 1,2$ here specifies one of the two nonequivalent sublattices of the copper (erbium) atoms, which occupy common fourfold positions of the space group $C^9_{2v}(Pna2_1)$: 1—(x_i,y_i,z_i); 2—$(\bar{x}_i,\bar{y}_i,1/2+z_i)$; 3—

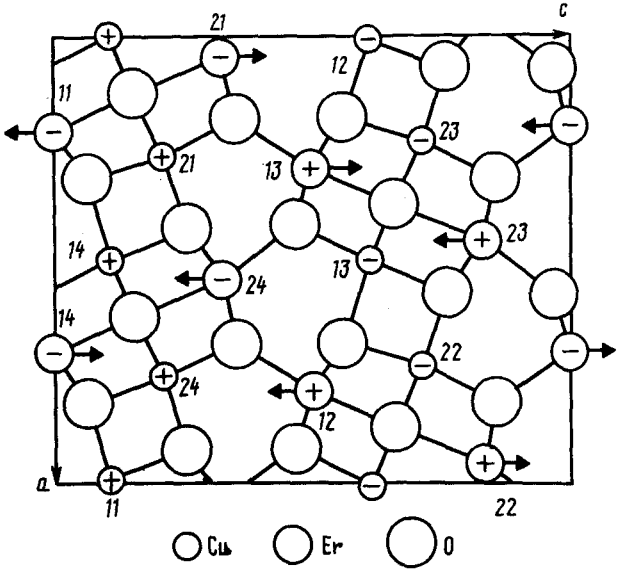

FIG. 1. Magnetic structure of $Er_2Cu_1O_5$. +, − (Components along the **b** axis; arrows) projections onto the **c** axis.

TABLE II.

M, μ_B \ T, K	1.9	16
Cu M_y	1.0 (1)	0.85 (8)
Er1 M_y	− 4.92 (4)	− 3.51 (5)
Er1 M_z	2.14 (6)	1.52 (8)
Er1 M	5.36 (5)	3.82 (6)
Er2 M_y	− 3.14 (7)	− 2.55 (7)
Er2 M_z	− 2.42 (6)	− 1.93 (6)
Er2 M	3.96 (7)	3.20 (7)

$(1/2 - x_i, 1/2 + y_i, 1/2 + z_i)$; 4—$(1/2 + x_i, 1/2 - y_i, z_i)$. In calculating the intensities of the magnetic reflections by the method of Ref. 3, we used the basis functions given above and the coordinates of the atoms [0.9908 0.6692 0.1121) for Cu1, (0.2603 0.6488 0.2140) for Cu2, (0.2064 0.2215 0) for Er1, (0.0401 0.2186 0.3297) for Er2] found through an interpolation between $Ho_2Cu_2O_5$ (Ref. 4) and $Lu_2Cu_2O_5$ (Ref. 5). (The number of nuclear reflections at our wavelength, $\lambda = 2.488$ Å, was too small for determining these coordinates with an adequate accuracy.) The intensity ratios show unambiguously that the Γ_1 representation holds over the entire temperature range 1.9 $K < T < T_N$. For this representation, the best theoretical values are compared with experimental values in Table I. For the Γ_2 representation we find $I_{003}/I_{201} \approx 3$, for Γ_3 we find $I_{003}/I_{201} = 0$, and for Γ_4 there should be no reflections at all (001, 201, 003,...) due to the **A(a)** mode.

The magnetic structure is shown in Fig. 1. The copper moments are directed along the **b** axis (A_1^y, A_2^y). The rare earth is polarized in the **bc** plane $(-a_1^y - a_2^y, -c_1^z, c_2^z)$. Table II shows the values of the components of the magnetic moments. We did not observe changes in the magnetic structure at the temperature $T_1 = 12$ K, which corresponds to the second susceptibility peak observed in Ref. 1. In addition, the relation between the components a^y and c^z remains the same above and below this temperature in both of the rare-earth sublattices. Only the values of the Er1 and Er2 moments vary with the temperature. Note the substantial difference between these moments and the difference in their behavior as a function of the temperature. These differences indicate a difference in the magnitude of the splitting of the ground doublet.

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