Neutron-powder-diffraction study of the structure and antiferromagnetic ordering in Pr_2CuO_4

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A neutron-powder-diffraction study has been carried out on Pr_2CuO_4, which has the T'-type structure of the new high-T_c electron superconductors. The compound orders antiferromagnetically at about 270 K. The magnetic intensities at 15 K can be equally well accounted for by a collinear magnetic structure with orthorhombic symmetry or a noncollinear structure with tetragonal symmetry. In both cases, Cu moments are coupled antiferromagnetically within the CuO_2 layers, the ordered moment being $0.48\mu_B$ at 15 K. Rietveld refinement at 298 and 15 K shows the crystal structure is essentially unchanged; in particular, there is no detectable distortion at low temperature.

INTRODUCTION

The discovery of high-temperature superconductivity in Cu-based mixed oxides has stimulated a great deal of interest in the magnetic properties of these compounds. Neutron-diffraction investigations on systems of this type, including La_2CuO_{4-y},[1-5] $YBa_2Cu_3O_{6+x}$,[6-12] $NdBa_2Cu_3O_{6+x}$.[7,13,14] $TlBa_2YCu_2O_7$,[15] and $Ca_{0.85}Sr_{0.15}CuO_2$,[16] have revealed the existence of long-range magnetic order in which near-neighbor Cu moments in the CuO_2 planes are coupled antiparallel. Measurements on single crystals of La_2CuO_{4-y} (Refs. 17–19) and $YBa_2Cu_3O_{6.2}$ (Ref. 20) have shown that the spins in these planes are well described in terms of a two-dimensional spin-$\frac{1}{2}$ Heisenberg model with strong exchange coupling within the planes. In doped crystals of $La_{2-x}Sr_xCuO_4$ with x between 0.2 and 0.18, the Néel state is destroyed, and the spin-spin correlation length decreases rapidly with increasing x but persists into the superconducting state.[21,22] A comprehensive account of this topic is given in a recent review article by Birgeneau and Shirane.[23]

The recent discovery of electron-type superconductivity in the system $L_{2-x}Ce_xCuO_{4-y}$, where L=Pr, Nd, or Sm,[24,25] has particularly interesting implications in view of the fact that in the previously known high-T_c materials the charge carriers are considered to be holes. Furthermore, these new compounds have the T'-type crystal structure of Nd_2CuO_4,[26] which differs in one important respect from the T-type structure of K_2NiF_4 and the distorted orthorhombic form found in La_2CuO_4 below about 500 K.[27] The rare-earth atoms, Cu, and one set of oxygen atoms are in similar positions, but the second set of oxygens are in sites above and below the oxygens in the CuO_2 planes instead of the apical positions occupied in the La_2CuO_4 structure (Fig. 1). The magnetic properties of this class of compounds are therefore likely to be of considerable interest in regard to the superconducting properties.[28]

Magnetic susceptibility and electron paramagnetic res-

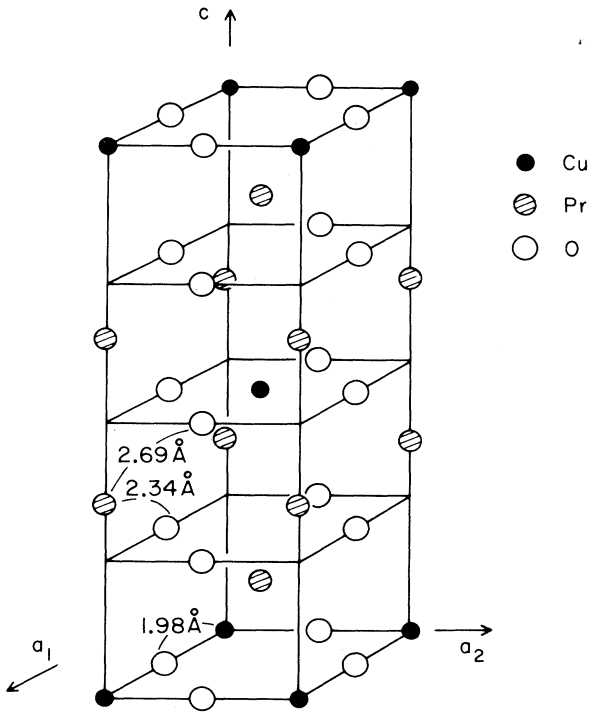

FIG. 1. T'-type structure of Pr_2CuO_4. Note the absence of oxygen at the apical positions above and below the Cu atoms.

onance measurements on polycrystalline samples of L_2CuO_4 (L=Nd, Pr, Eu, and Gd) have been reported by Saez Puche and co-workers,[29,30] who concluded that the Cu moments were ordered antiferromagnetically below 300 K. Recent muon spin-rotation experiments on the Nd, Pr, and Sm compounds have confirmed that antiferromagnetic ordering of the Cu moments occurs for all three materials in the region of 250–300 K, and antiferromagnetic order was also observed in a partially doped, nonsuperconducting material of composition $Nd_{1.9}Ce_{0.1}CuO_{4-y}$ but not in superconducting $Nd_{1.84}Ce_{0.16}CuO_{4-y}$.[31] In addition, magnetization measurements on single crystals indicate ordering of the Cu moments in Gd_2CuO_4 at about 260 K and possibly in Eu_2CuO_4 near 245 K.[32]

The present paper describes the results of a neutron-powder-diffraction investigation of the magnetic ordering in a polycrystalline sample of Pr_2CuO_4 with a Néel temperature of around 270 K.[33]

EXPERIMENTAL DETAILS

The sample was prepared by heating a stoichiometric mixture of Pr_2O_3 and CuO in air at 1100 °C for 24 h. An x-ray-powder-diffraction pattern showed the expected tetragonal phase.

Unpolarized neutron measurements were made at the Brookhaven High Flux Beam Reactor on a triple-axis diffractometer equipped with a pyrolytic graphite monochromator and analyzer in the (002) setting scattering at a wavelength of 2.371±0.001 Å. The collimation was 20′ in-pile, 40′ monochromator sample, 40′ sample analyzer, and 20′ analyzer detector. Higher-order harmonics were suppressed by a pyrolytic graphite filter. Polarized-beam measurements were carried out on a second triple-axis machine equipped with a Heusler alloy monochromator and analyzer in the (111) setting set up to measure the cross section for spin-flip (magnetic) scattering at a wavelength of 2.35 Å with collimation 40′ 80′, 80′, and about 130′ in the positions specified above. Intensity measurements were made with a magnetic field applied first parallel (horizontal) and then perpendicular (vertical) to the scattering vector. The difference between the intensities obtained with the horizontal (HF) and vertical (VF) configurations is proportional to one-half of the magnetic cross section measured in the unpolarized beam, and the background and any residual nuclear scattering cancel out. A detailed description of the polarized-beam technique has been given elsewhere.[34,35]

The sample was loaded into an Al holder and placed in a closed-cycle He cryostat for temperature-dependence measurements. Extended data sets suitable for structure refinement were collected with unpolarized neutrons at 298 and 15 K by step scanning at 0.1° intervals over the angular range 18–118°. Shorter scans were performed over selected regions at intermediate temperatures.

RESULTS

At 298 K the expected tetragonal pattern was observed, together with one unindexed weak peak with a d spacing of 1.93 Å and a relative intensity about 1% of that of the strongest Pr_2CuO_4 peak. At 15 K a few more weak peaks were seen which could be indexed with half-

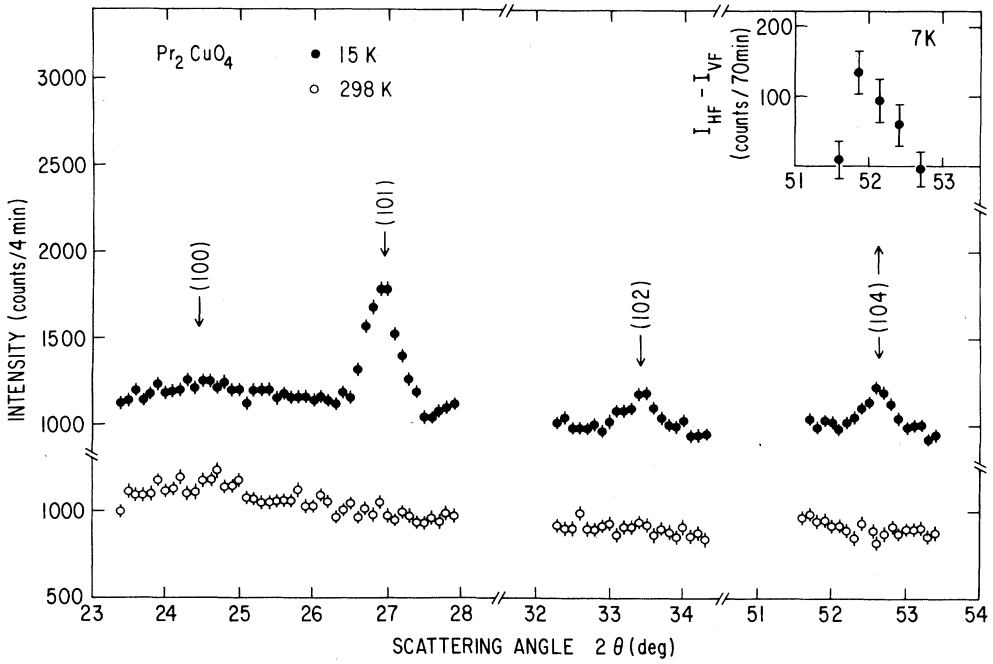

FIG. 2. Scans over regions around selected magnetic peaks for Pr_2CuO_4 at 298 and 15 K. The inset shows the difference between polarized-beam measurements in horizontal and vertical magnetic fields for the (104) reflection at 7 K.

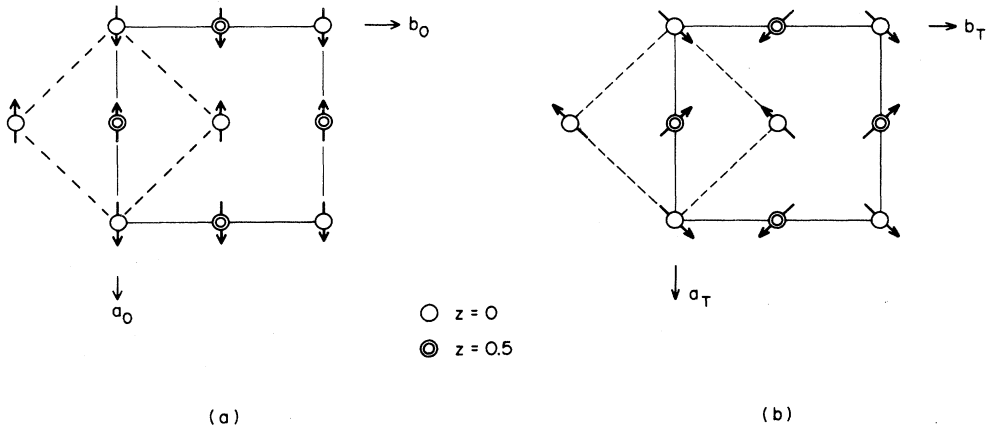

FIG. 3. Alternative magnetic structures for Pr_2CuO_4 at 15 K as described in text. (a) Collinear, orthorhombic symmetry ($F_Amm'm'$); (b) noncollinear, tetragonal symmetry ($P4_2/nc'm'$).

integer values of h and k, corresponding to an enlarged cell with lattice parameters $a\sqrt{2},c$. In the following description the magnetic peaks are indexed in terms of this enlarged cell. The corresponding reflection conditions are then $h+k$ odd, analogous to the magnetic peaks observed in La_2CuO_4 and indicative of antiferromagnetic ordering within the CuO_2 planes. A few of these peaks are illustrated in Fig. 2, which shows scans of selected regions taken with good counting statistics at 15 and 298 K. The strongest peak is (101); however, (100) is seen to be absent, although there is an indication of diffuse scattering in this region which does not change much with temperature.

TABLE I. Comparison of calculated and observed magnetic intensities for Pr_2CuO_4 at 15 K. Model 1 is the collinear structure of Fig. 3(a) (magnetic space group $F_Amm'm'$), model 2 is the noncollinear structure of Fig. 3(b) ($P4_2/nc'm'$). In the latter case, hkl and khl reflections are equivalent, as required by tetragonal symmetry, and the calculated intensities are combined. The Cu moment is $0.48\mu_B$, as calculated from the (011) intensity and the nuclear scaling factor obtained from the Rietveld refinement in Table II. Calculated magnetic form factor for Cu^{2+} obtained from Ref. 39. Numbers in parentheses represent maximum estimated uncertainties in observed intensities.

Reflection	Model 1 I(calc)	Model 2 I(calc)	I(obs)
100			0(3)
010			
101		18.5	37(3)
011	37	18.5	
102	10	5	10(3)
012		5	
103		6.5	9(4)
013	13	6.5	
104	6	3	9(3)
014		3	
210		2.5	4(2)
120	5	2.5	
211	3	1.5	8(4)
121		1.5	

Polarized neutron measurements made at 50 K at the (101) peak position confirmed that the scattering was magnetic in origin. In addition, a short scan was performed across the (104) peak, which in the case of La_2CuO_4 is predominantly nuclear in origin due to the orthorhombic distortion. The difference between the horizontal- and vertical-field intensities ($I_{HF}-I_{VF}$) at 7 K is shown in the inset to Fig. 2. A comparison with the nuclear intensities shows that these magnetic intensities are consistent with those observed in the unpolarized-beam measurements.

At first sight the observed magnetic peaks together with the absence of any scattering at the (100) position indicate an antiferromagnetic structure consisting of ferromagnetic (100) sheets of moments coupled antiparallel to adjacent sheets similar to those in La_2CuO_4 but with the moments directed along the [100] axis rather than the [010] axis, i.e., perpendicular to the sheets. This struc-

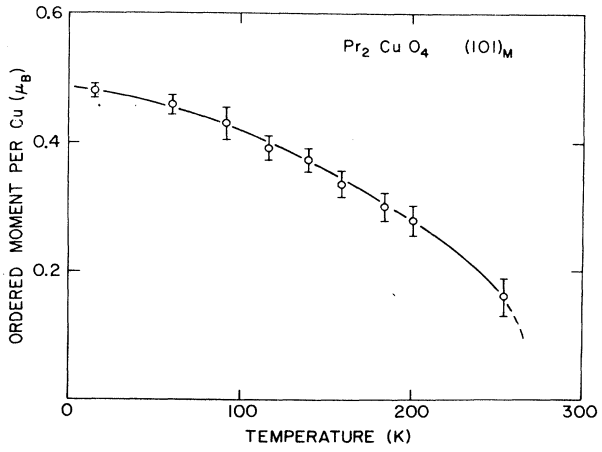

FIG. 4. Ordered moment of Cu as a function of temperature. T_N is estimated to be 270±10 K.

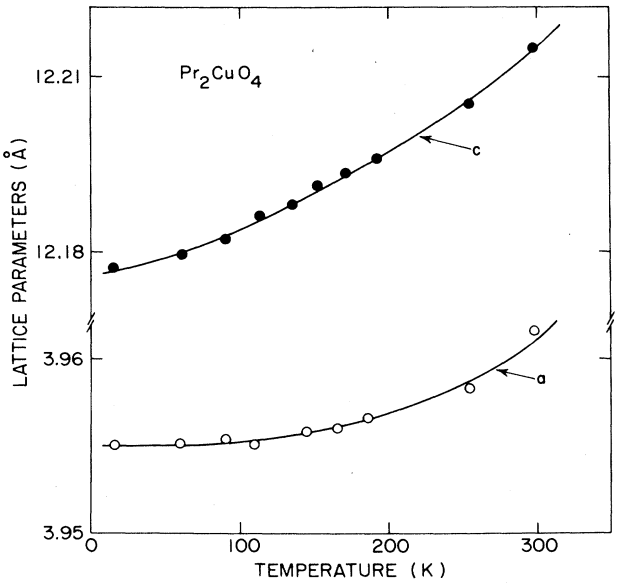

FIG. 5. Lattice parameters of Pr_2CuO_4 as a function of temperature.

ture is shown in projection in Fig. 3(a) and is identical to that reported for $La_2NiO_{4.05}$ (Refs. 36 and 37) and the high-temperature magnetic structure of La_2CoO_4.[38] Observed and calculated magnetic intensities based on this model and a Cu moment of $0.48\pm0.03\mu_B$ are in reasonable agreement (Table I, model 1).

The temperature dependence of the ordered moment was determined from the variation of the intensity of the magnetic (101) reflection, as shown in Fig. 4. From this the Néel temperature is estimated to be 270 ± 10 K, in agreement with the muon experiments.[3]

The variation of the lattice parameters between 15–300 K was determined from least-squares fits to scans taken over the tetragonal (008) and (200) peaks, as illustrated in Fig. 5. Although the magnetic structure depicted in Fig. 3 clearly has orthorhombic symmetry there is no detectable splitting or broadening of the tetragonal (220) peak which would signal an orthorhombic distortion of the type observed in La_2CuO_4. If a small orthorhombic distortion in fact exists, the corresponding strain $(b-a)/(b+a)$ is estimated to be no more than 1×10^{-3}. The alternative possibility of a noncollinear structure with tetragonal symmetry should, therefore, be considered.

Based on magnetic symmetry arguments[40] a structure of this type can be derived [Fig. 3(b)] which gives calculated intensities (Table I, model 2) identical to those of the orthorhombic structure (Table I, model 1). The corresponding magnetic symmetry is $P4_2/nc'm'$, and the structure can be viewed as a coherent superposition of the structure in Fig. 3(a) (magnetic symmetry $F_Amm'm'$) and its 90° counterpart. This sort of degeneracy is a familiar problem in magnetic-structure analysis from neutron powder data and is difficult to resolve without a single crystal which is predominantly one domain.

Rietveld refinement of the 298 K data set was carried out in space group $I4/mmm$ with a modified version of the Rietveld-Hewat program.[41,42] Background values were obtained by linear interpolation between intensities averaged over regions between peaks. Gaussian peak shapes were assumed and intensities calculated over a total angular range of four full widths at half maximum. The number of peaks was 18, and the variable parameters included the z parameter of Pr, four individual isotropic temperature factors, and six profile variables (half widths, unit cell parameters, and a zero-point correction). Analysis of the 15 K data set was carried out in the same way, except that the magnetic peaks were included and the Cu moment was refined. The results are listed in Table II, and the profile fits are illustrated in Fig. 6. Both fits are very satisfactory, as indicated by the R factors and goodness-of-fit indices in Table II and the difference plots in Fig. 6. In particular, there are no anomalously high temperature factors indicative of static displace-

TABLE II. Refined values of structural parameters for Pr_2CuO_4 at 298 and 15 K. Scattering amplitudes for Pr, Cu, and O taken as 0.445, 0.7718, and 0.5805×10^{-12} cm, respectively (Ref. 43). Numbers in parentheses are estimated standard deviations and refer to the least significant digit. R_I, R_{wp}, R_e, S_p^2, and S_I^2 are defined in Ref. 44.

		298 K				15 K			
Atom	Site	x	y	z	B(Å^2)	x	y	z	B(Å^2)
Pr	4(e)	0.0	0.0	0.3512(2)	0.2(1)	0.0	0.0	0.3517(1)	0.1(1)
Cu	2(a)	0.0	0.0	0.0	0.6(1)	0.0	0.0	0.0	0.3(1)
O(1)	4(c)	0.0	0.5	0.0	0.4(1)	0.0	0.5	0.0	0.2(1)
O(2)	4(d)	0.0	0.5	0.25	0.3(1)	0.0	0.5	0.25	0.2(1)
	a (Å)			3.9615(1)				3.9550(1)	
	c (Å)			12.2140(5)				12.1772(3)	
	Moment (μ_B)							0.48(1)	
	R_I			0.012				0.009	
	R_{wp}			0.065				0.045	
	R_e			0.030				0.027	
	S_p^2			4.8				2.8	
	S_I^2			5.9				4.0	

ments as found in some of these materials. An attempt to refine the occupancies of the O(1) and O(2) sites gave values slightly, but not significantly, greater than unity [1.02(1) in both cases]. A similar refinement as the apical site position of the O(2) atom in the La_2CuO_4 structure yielded a value of 0.00(1). Thus the compound is stoichiometric within the accuracy of the refinement, and there is no evidence of any disorder. The 298 K results are in good agreement with those reported for an earlier sample of this material.[45]

DISCUSSION

The structure of Pr_2CuO_4 is shown in Fig. 1. Each Cu has four O neighbors in square planar coordination at a distance of 1.98 Å, and Pr has eight O neighbors in a dis-

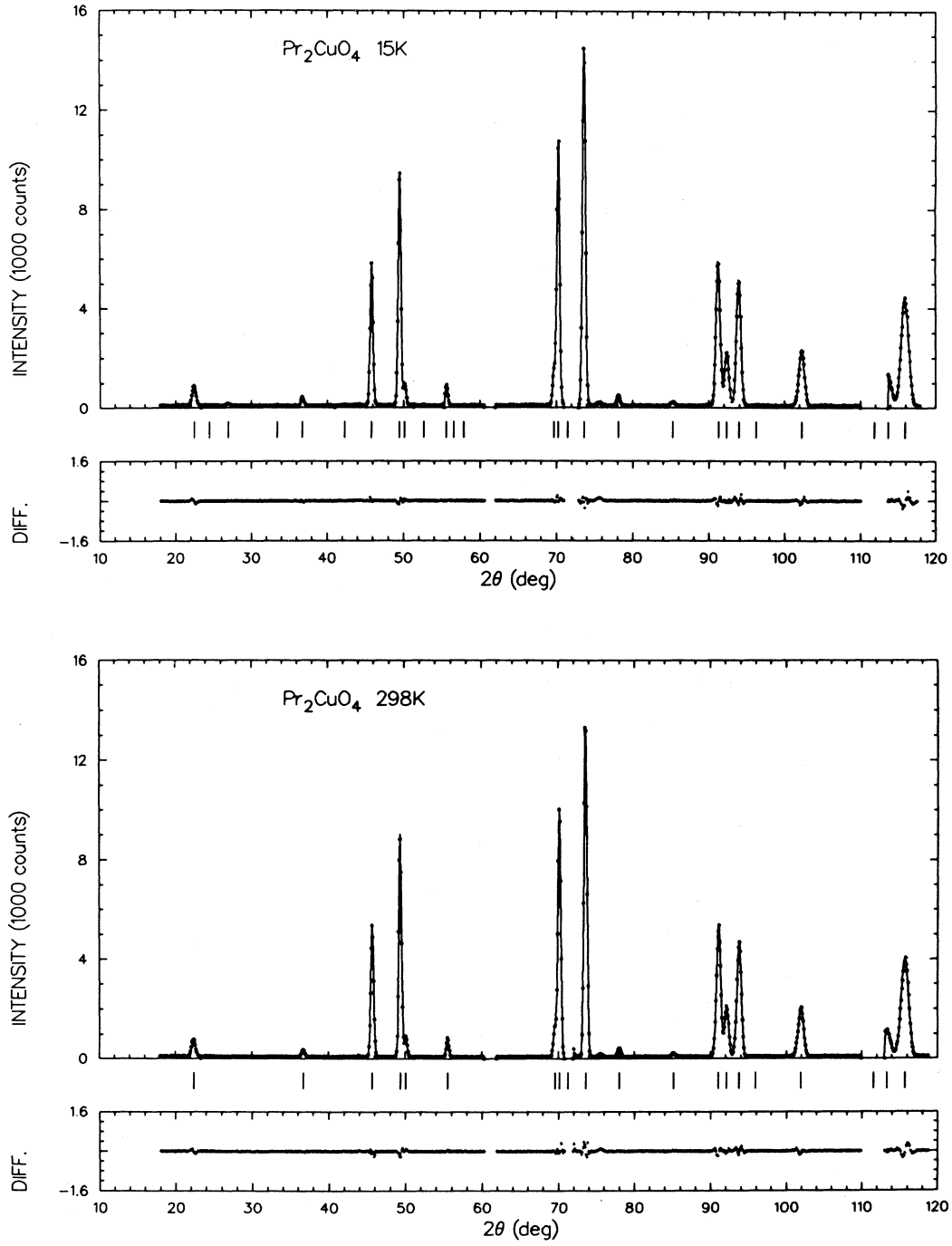

FIG. 6. Profile fits and difference plots for Pr_2CuO_4 at 15 K (top) and 298 K (bottom). Short vertical markers represent allowed reflections. The extra reflections at 15 K are magnetic peaks. Sample holder peaks have been excluded.

torted cubic environment, four at 2.69 Å and four at 2.34 Å.

The data obtained in the present study show no striking differences in the magnetic behavior of Pr_2CuO_4 and La_2CuO_4. The magnetic structure of the former is consistent with strong antiferromagnetic coupling within the CuO_2 planes, and the similar Néel temperatures indicate that the weak interplanar interactions responsible for three-dimensional order are comparable in spite of the differences in oxygen coordination.

As discussed above, it is not possible to rule out a noncollinear array of moments in Pr_2CuO_4. A related model of this type has also been suggested for the low-temperature magnetic structure of La_2CoO_4, which undergoes a first-order crystallographic phase transition from orthorhombic to tetragonal symmetry at about 135 K.[38] This transition is accompanied by the appearance of a magnetic (100) reflection and an abrupt decrease in the intensity of the orthorhombic (011) peak. The noncollinear structure would then be the coherent superposition of two structures of La_2CuO_4 type. An analogous crystallographic phase transition has been observed in the $La_{2-x}Ba_xCuO_4$ system for values of x between 0.05 and 0.20.[46] The proposed driving mechanism is a softening of the second rotational mode of the oxygen octahedra which results in a change from *Bmab* to $P4_2/ncm$ symmetry. In this the octahedra rotate about alternate tetragonal ⟨100⟩ axes from layer to layer. If the true low-temperature symmetry of Pr_2CuO_4 were $P4_2/ncm$, there would be two sets of O(1) sites, 4(a) at $\frac{3}{4}$, $\frac{1}{4}$, 0, and 4(e) at $\frac{1}{4}$, $\frac{1}{4}$, z, with $z=0.0$, and likewise for O(2), 4(b), at $\frac{3}{4}$, $\frac{1}{4}$, $\frac{1}{4}$, and 4(e) at $\frac{1}{4}$, $\frac{1}{4}$, z, with $z\approx 0.25$. Slight shifts in the z coordinates from the ideal values would lead to a buckling of the oxygen sheets and the appearance of weak nuclear superlattice peaks. However, any such shifts must be very small, since no extra nuclear peaks were observed in the present experiment. It would be of interest to check this point by a single-crystal investigation.

It is interesting to note that antiferromagnetic ordering of the Pr moments in $PrBa_2Cu_3O_7$ has recently been observed below 17 K with a saturation value of $0.24\mu_B$.[47] The intensities in Table II are not consistent with any similar ordering in Pr_2CuO_4 at 15 K in excess of a moment of about $0.05\mu_B$.

ACKNOWLEDGMENTS

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