JOURNAL OF SOLID STATE CHEMISTRY 79, 285–287 (1989)

Magnetic Structure of $PrCrOS_2$

M. WINTENBERGER, VOVAN TIEN, M. GUITTARD, AND J. DUGUÉ

Laboratoire de Chimie Minérale Structurale, Unité Associée au CNRS No. 200, Faculté des Sciences Pharmaceutiques et Biologiques de Paris–Luxembourg, 4 Avenue de l'Observatoire 75270 Paris Cedex 06, France

Received October 12, 1988

$PrCrOS_2$ is antiferromagnetic with $T_N = 83$ K. The magnetic space group is B_p2'/m'. The variations of μ_{Cr} and μ_{Pr} with temperature were studied. The properties of $PrCrOS_2$ are very similar to those of $NdCrOS_2$. © 1989 Academic Press, Inc.

$PrCrOS_2$ belongs to a group of compounds $LnCrOX_2$ (Ln = La to Nd and X = S or Se) which are characterized by the presence of $(LnO)_n$ double chains (*1*, *2*).

In previous papers (*3*, *4*) we reported the magnetic properties and magnetic structures of La and Nd compounds. The present paper describes the study of $PrCrOS_2$.

The method of preparation is the same as for $LaCrOS_2$ (*3*). $PrCrOS_2$ is isomorphous to $CeCrOS_2$ and $NdCrOS_2$. The space group is $B2/m$. Cr_I and Cr_{II} are respectively on sites 2a and 2d, and Nd is on site 4i. The parameters are $a = 1.15$, $b = 0.80$, $c = 0.37$ nm, $\gamma = 90°2$.

The X-ray powder diagrams of the three oxysulfides are practically identical, and single crystal refinements of the structures of the Ce and Nd compounds give the same atomic coordinates, so we took the same values for $PrCrOS_2$.

Susceptibility measurements were made with a vibrating sample magnetometer in fields up to 2 tesla.

The $\chi^{-1}(T)$ curve is shown in Fig. 1. $PrCrOS_2$ is antiferromagnetic, with a Néel temperature $T_N = 83$ K.

Neutron diffraction spectra were recorded at several temperatures on the 800 cell powder diffractometer at Laboratory Léon Brillouin.[1] The wavelength was 0.246 nm.

From the 5 K spectrum it is easily concluded that the magnetic structure is similar to that of $NdCrOS_2$ (Fig. 2). The space group is B_p2'/m', the moments being in (001) planes. The only difference between the two structures is that for $PrCrOS_2$ we get a better fit with moments at 15° from the b axis in the a, b quadrant, whereas they were found along the b axis in $NdCrOS_2$.

[1] Laboratoire commun CEA–CNRS.

0022-4596/89 $3.00

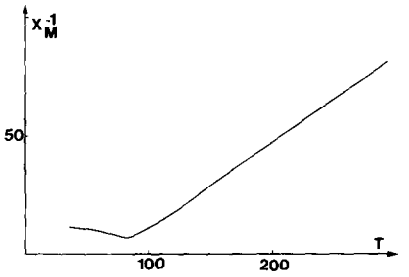

FIG. 1. Inverse molar susceptibility of $PrCrOS_2$ versus T.

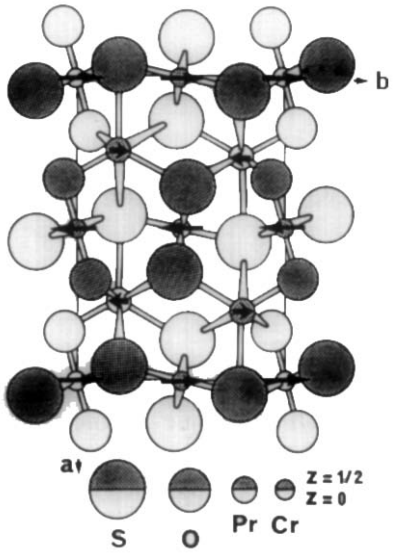

FIG. 2. Magnetic structure of $PrCrOS_2$.

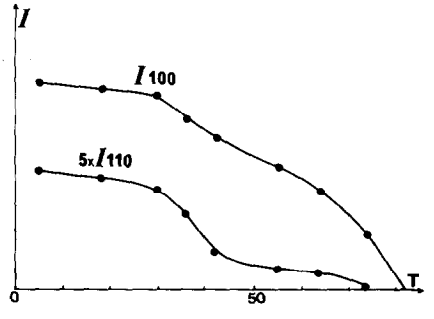

FIG. 3. Temperature dependence of the intensities of (100) and (110) reflections.

TABLE I

OBSERVED (NONCORRECTED FOR THE LORENTZ FACTOR) AND CALCULATED INTENSITIES OF $PrCrOS_2$ AT 5 K

$h\,k\,l$	I_{calc}	I_{obs}
	Nuclear reflections	
010	9.06	8.
200	0.65	0.49
$210/2\bar{1}0$	3	2.8
020	1.96	2.3
101	0.225	0.14
	Magnetic reflections	
	$h + k = 2n$	
$110/1\bar{1}0$	6.4	5.7
001	3.3	3.2
$310/3\bar{1}0$	3.9	4.65
201	4.5	4.5
021	1.5	1.8
$130/1\bar{3}0$	0.3	—
	$h + k = 2n + 1$	
100	46.5	47.2
300	2.36	1.5
$120/1\bar{2}0$	2.34	3
011	4.15	2.2
$211/2\bar{1}1$	9.2	8.3
$320/3\bar{2}0$	1.74	2.2

Note. $\mu_{Cr} = 2.6\ \mu_B$; $\mu_{Pr} = 2.25\ \mu_B$. Moments at 15° from b axis in the a, b quadrant.

Actually we assumed that the moments of Cr_I, Cr_{II}, and Pr all have the same direction, although this is not required by symmetry arguments, because we do not have enough data to refine a model with small angles between the three moments.

The observed and calculated nuclear and magnetic intensities are given in Table I. For Pr we used the experimental form factor of Lebech *et al.* (*5*). We found $\mu_{Cr} = 2.6\ \mu_B$ and $\mu_{Pr} = 2.25\ \mu_B$ at 5 K.

The variation of the magnetic intensities with temperature (Fig. 3) is also very similar to that of $NdCrOS_2$ and shows in the same way that the Cr–Pr exchange interaction is a nonnegligible fraction of the one for Cr–Cr.

Acknowledgments

We thank Y. Allain and G. André of Laboratory Léon Brillouin for their help during the neutron experiments.

References

1. J. DUGUÉ, VOVAN TIEN, AND J. VILLERS, *Acta Crystallogr. Sect. B* **36,** 1291–1294 (1980).
2. J. DUGUÉ, VOVAN TIEN, AND J. VILLERS, *Acta Crystallogr. Sect. B.* **36,** 1294–1297 (1980).
3. M. WINTENBERGER, VOVAN TIEN, AND M. GUITTARD, *Solid State Commun.* **53,** 227–230 (1985).
4. M. WINTENBERGER, J. DUGUÉ, M. GUITTARD, NGUYEN HUY DUNG, AND VOVAN TIEN, *J. Solid State Chem.* **70,** 295–302 (1987).
5. B. LEBECH, B. D. RAINFORD, P. J. BROWN, AND F. A. WEDGWOOD, *J. Magn. Magn. Mater.* **14,** 298–300 (1979).