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A SIMPLE MAGNETIC MODEL FOR $PrCu_5$

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Abstract

A simple magnetic model for $PrCu_5$ is proposed. The two basic features are: 1) a simplified singlet-triplet crystal field splitting extracted from the nine level scheme ($J = 4$ for Pr^{+3}) of the actual crystal field levels given in the literature and 2) a molecular field approximation of the exchange interaction between the Pr^{+3} ions. A magnetic state equation is derived and a best fitting analysis of the magnetic susceptibility given in the literature is performed. We also discuss the combined role of exchange and crystal field on the onset of magnetic order.

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The crystal field splitting of Pr^{+3} in $PrCu_5$ has been investigated by A. Andreef et al /1/. The crystal field parameters were then used to analyse magnetic properties, in particular the temperature dependence of the inverse of the susceptibility.

In this paper we present a simple model for the computation of the inverse of the susceptibility of $PrCu_5$. We take into account only the two lowest levels of the crystal field given in reference /1/, and construct an effective Hamiltonian containing the simplified crystal field and a Heisenberg exchange in a molecular field approximation.

The model Hamiltonian is

$$H = H_{CEF} + H_{MAG} \tag{1}$$

where H_{CEF} and H_{MAG} in matrix notation are

$$H_{CEF} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \Delta & 0 \\ 0 & 0 & \Delta \end{pmatrix} \tag{2}$$

$$H_{MAG} = -\mu_B h_i \begin{pmatrix} 0 & \alpha_0 & \alpha_0 \\ \alpha_0 & 0 & 0 \\ \alpha_0 & 0 & 0 \end{pmatrix} \tag{3}$$

Expressions 2 and 3 are constructed taking into account only the two lowest levels of the nine states of Pr^{+3} in a hexagonal symmetry. The wave functions of these levels are

$$\Gamma_1 = |e_0\rangle = |0\rangle \tag{4-a}$$

$$\Gamma_6 \begin{cases} |e_1\rangle = |-1\rangle & \text{(4-b)} \\ |e_2\rangle = |1\rangle & \text{(4-c)} \end{cases}$$

In expression 2 Δ is the energy difference between the Γ_1 and Γ_6 levels. Since the easy magnetization is in the x-direction

$$\mathcal{H}_{mag} = - \mu_B h_i g J_x \tag{5}$$

where J_x is the x-component of the total angular momentum ($J = 4$), μ_B is the Bohr magneton and g an effective Lande-factor. Using the basis given in 4, expression 3 is obtained where

$$\alpha_0 = \langle e_0|gJ_x|e_1\rangle = \langle e_0|gJ_x|e_2\rangle \tag{6}$$

In what follows we take α_0 as a free parameter.

In 5, h_i is an exchange molecular field plus an external magnetic field h_0

$$\mu_B h_i = J_0\langle gJ_x\rangle + \mu_B h_0 \tag{7}$$

where $J_0 = \dfrac{zj(g-1)^2}{g^2}$ and z is the number of nearest neighbours Pr^{+3} to a given Pr^{+3} and j is the exchange interactions between two Pr^{+3} ions.

In order to compute the magnetic susceptibility we calculate a magnetic state equation using

$$M = \sum_{n=0}^{2} f_n\left(- \frac{dE_n}{dh_i}\right) \tag{8}$$

where M is the magnetic moment per ion, E_n are the eigenvalues of (1) and

$$f_n = \frac{\exp(\beta E_n)}{\sum_n \exp(\beta E_n)} \tag{9}$$

with $\beta = \frac{1}{k_B T}$

The final expression for the temperature dependence of the magnetization is

$$M = \frac{4\alpha_0^2\mu_B^2 h_i}{\sqrt{\Delta^2+8\alpha_0^2(\mu_B h_i)^2}} \left\{ \frac{2\sinh\left[\frac{\beta(\Delta^2+8\alpha_0^2(\mu_\beta h_i)^2}{2}\right]^{1/2}}{\exp\left(-\frac{\beta\Delta}{2}\right) + 2\cosh\left[\frac{\beta(\Delta^2+8\alpha_0^2(\mu_B h_i)^2}{2}\right]^{1/2}} \right\} \tag{10}$$

From 10 we obtain the ionic magnetic susceptibility

$$x = \lim_{h_0 \to 0} \frac{M}{h_0} \tag{11}$$

we obtain

$$x = \frac{\frac{4\alpha_0^2\mu_B^2}{\Delta}\left[\frac{2\sinh(\beta\Delta/2)}{\exp(-\beta\Delta/2) + 2\cosh(\beta\Delta/2)}\right]}{1 - \frac{4\alpha_0 J_0}{\Delta}\left[\frac{2\sinh(\beta\Delta/2)}{\exp(-\beta\Delta/2) + 2\cosh(\beta\Delta/2)}\right]} \tag{12}$$

Equation 12 is valid for $T > T_c$, if the system presents spontaneous magnetic order.

From equation 10, at T = 0, with $h_0 = 0$ we obtain

$$\frac{M_0}{\mu_B} = \frac{\sqrt{2}\ \alpha_0(\eta^2-1)^{1/2}}{\eta} \tag{13}$$

where

$$\eta = \frac{4\alpha_0^2 J_0}{\Delta} \tag{14}$$

The onset of spontaneous magnetic order is obtained for $\eta = 1$.

We now apply the results obtained to the study of $PrCu_5$ for which (Andreef et al. /1/ investigated the temperature dependence of the magnetic susceptibility. From reference /1/ we take $\Delta = 3.23$ meV and using equation 12 we try to adjust the experimental points of the inverse magnetic susceptibility given in [1]. Making a best fitting analysis we get $\alpha_0 = 6.66$ and $J_0 = 0.008$ meV. The figure shows the experimental points of reference 1 and the solid curve is constructed using equation 12.

In this paper we have presented a simple magnetic model involving exchange and crystal field interactions. The crystal field effects are described in a reduced set of levels. As a consequence we obtain an analytic state equation which shows the role of exchange and crystal field parameters in determining the magnetic properties. Usually one has to describe the crystal field Hamiltonian using Stevens operators /2/ and to take into account the local symmetry of the crystal field; the final crystal field Hamiltomian is than expressed in the Lea-Leask-Wolf notation /3/. The task of obtaining magnetic quantities from a complete crystal field combined with a molecular field approximation for the exchange interaction can usually be obtained only numerically.

Figure Caption

Fig. 1 - Temperature dependence of the inverse of the susceptibility (in mol/emu) for $PrCu_5$. The full curve is computed from the parameters given in the text and the experimental points are taken from reference [1].

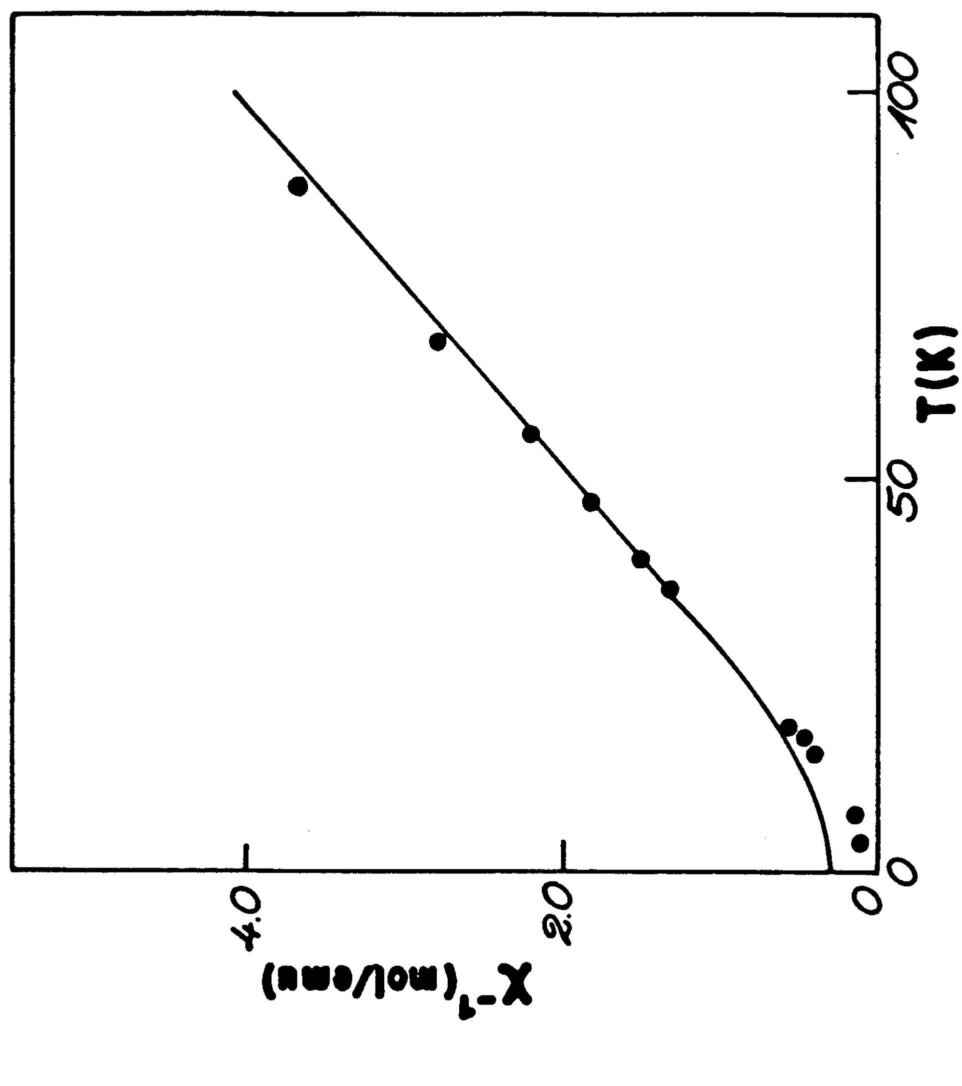

Fig. 1

Reference

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