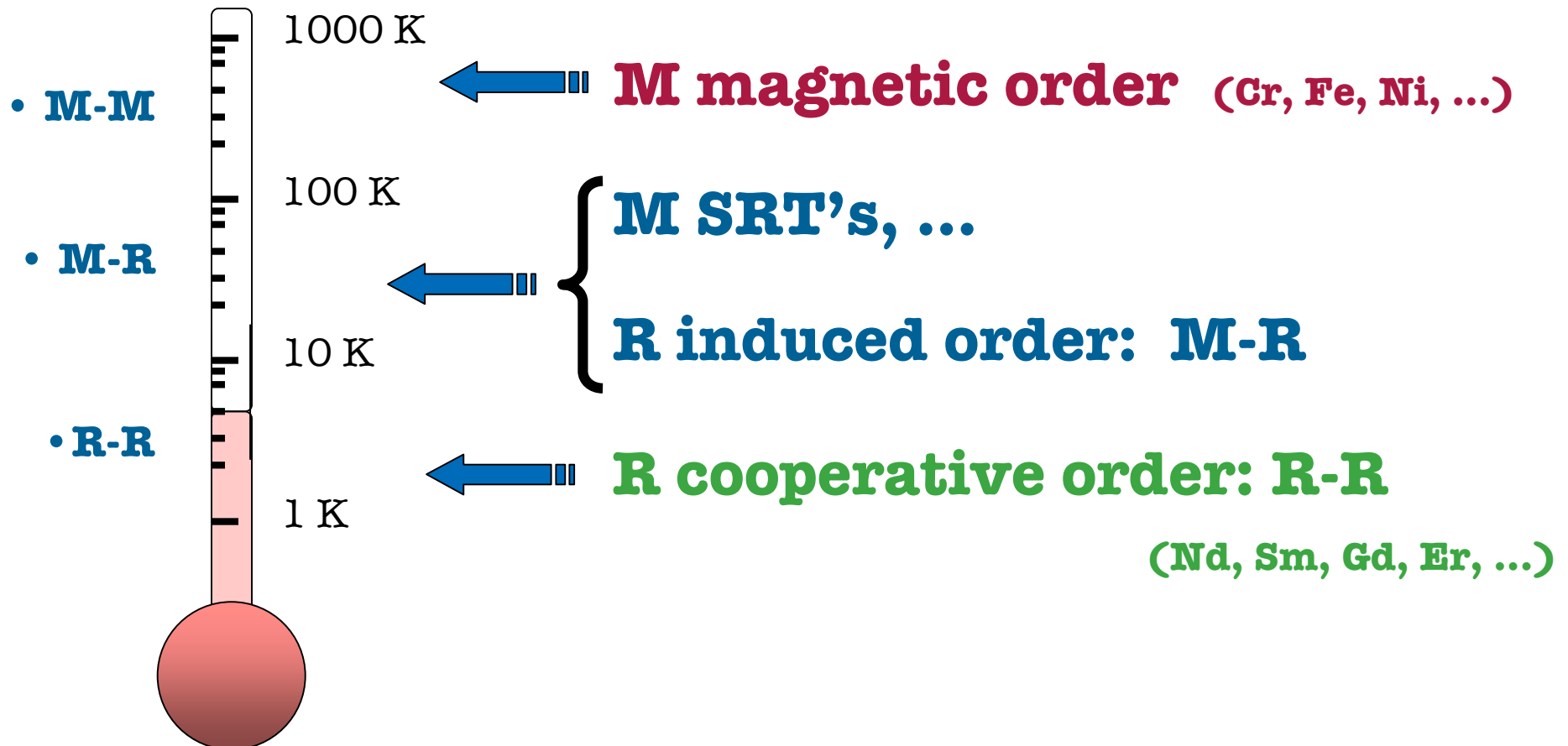
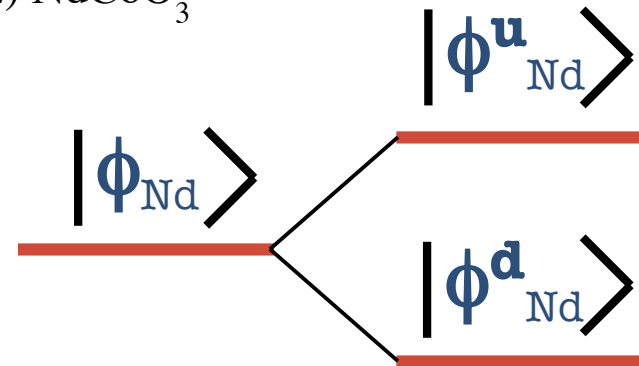
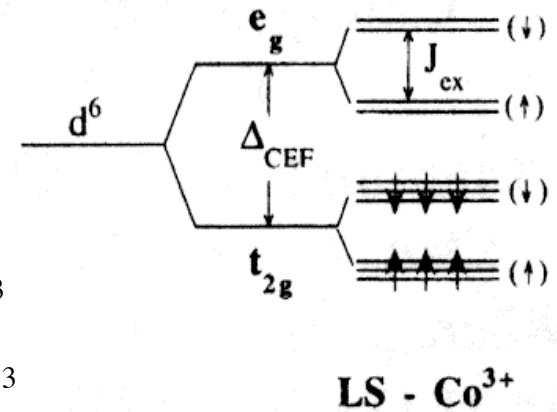
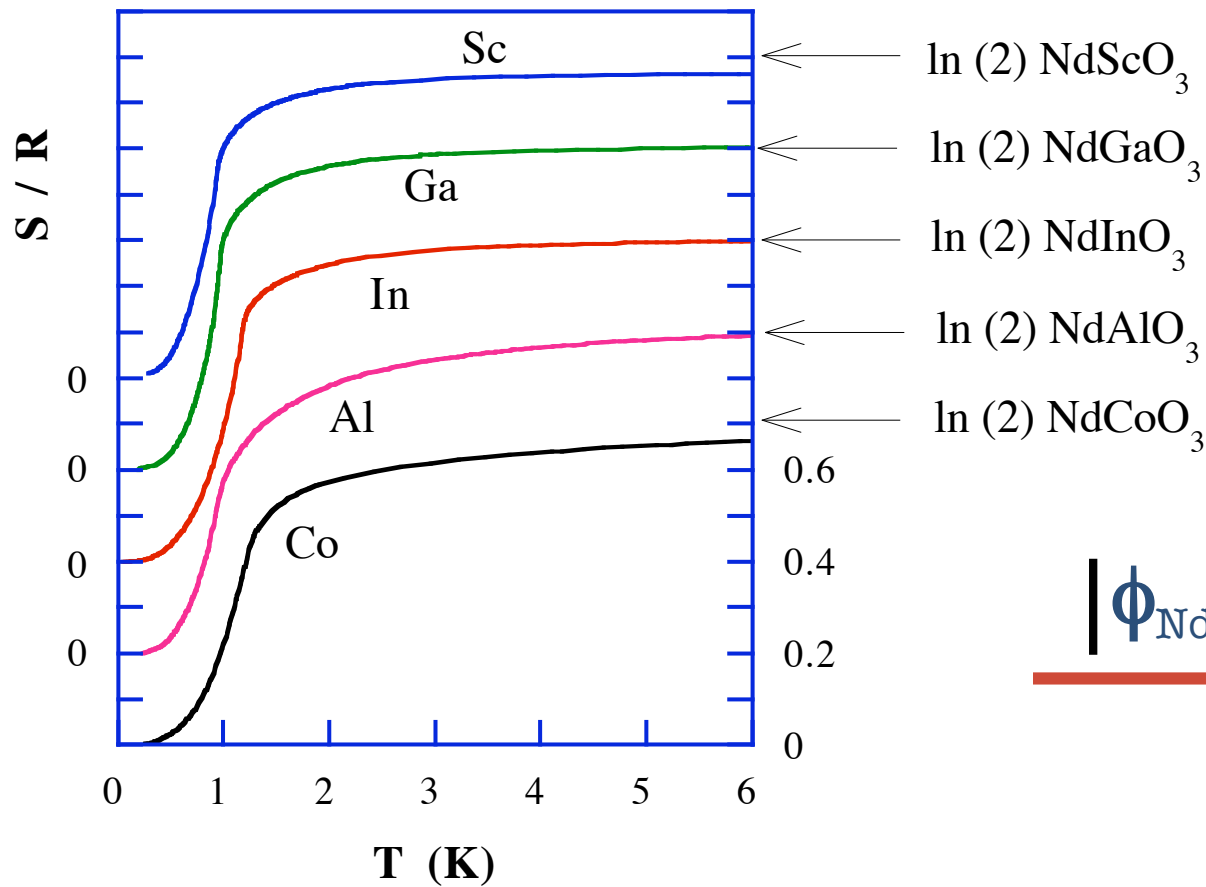


1. Introduction
2. Low-temperature Specific Heat results in  $\text{NdFe}_{1-x}\text{Co}_x\text{O}_3$  ( $x \leq 0.5$ )
3. Models and interpretation
4. Conclusions

**$\text{RMO}_3$**  : Model systems M-M, M-R, R-R interactions.



**$x=1$**  Co is in LS state in  $\text{NdCoO}_3$



## Magnetic susceptibility of NdGaO<sub>3</sub> at low temperatures: A quasi-two-dimensional Ising behavior

F. Luis, M. D. Kuz'min, F. Bartolomé, V. M. Orera, and J. Bartolomé

*Instituto de Ciencia de Materiales de Aragón, CSIC-Universidad de Zaragoza, Plaza San Francisco S/N, 50009 Zaragoza, Spain*

M. Artigas and J. Rubín

*Departamento Ciencia y Tecnología de Materiales y Fluidos, CPS and I.C.M.A., 50015 Zaragoza, Spain*

(Received 3 February 1998)

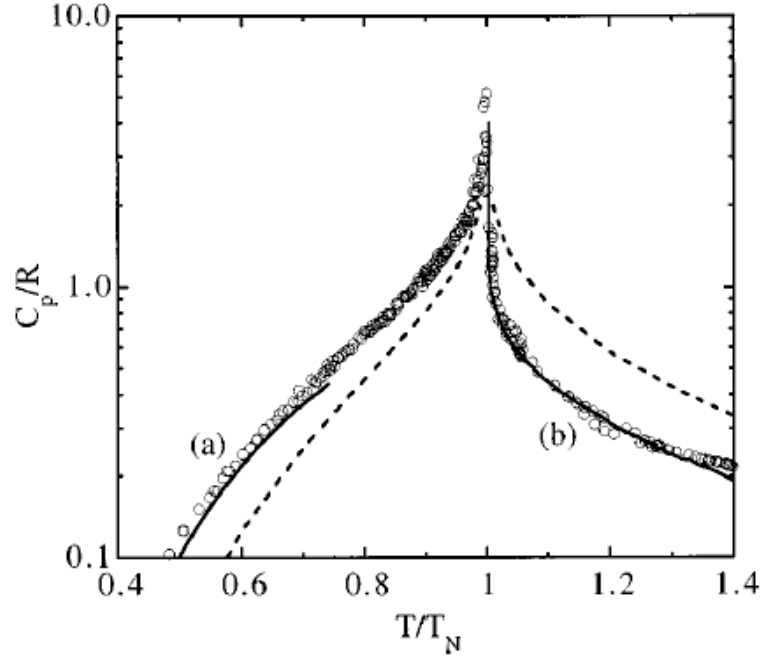


FIG. 9. Experimental heat capacity of NdGaO<sub>3</sub> vs reduced temperature ( $T_N=0.97$  K). (—) Calculated predictions for the 2D-3D crossover case with  $|r|=0.1$  from (a) spin-wave low-temperature series, (b) extrapolated high-temperature series. (---) Heat capacity for the antiferromagnetic simple quadratic  $S=\frac{1}{2}$  model ( $r=0$ ).

The heat capacity was calculated as

$$C/R = A \left( 1 - \frac{K}{K_c} \right)^{-\alpha} + e_0 + PA \left\{ \sum_{n=2}^{\infty} (K/2)^n \left( \sum_{j=0}^n c_{nj} r^j \right) - \left[ A \left( 1 - \frac{K}{K_c} \right)^{-\alpha} + e_0 \right] \right\} \quad (14)$$

above  $T_c = T_N$ , as shown in Fig. 9. We observe an excellent

## Magnetic susceptibility of NdGaO<sub>3</sub> at low temperatures: A quasi-two-dimensional Ising behavior

F. Luis, M. D. Kuz'min, F. Bartolomé, V. M. Orera, and J. Bartolomé

*Instituto de Ciencia de Materiales de Aragón, CSIC-Universidad de Zaragoza, Plaza San Francisco S/N, 50009 Zaragoza, Spain*

M. Artigas and J. Rubín

*Departamento Ciencia y Tecnología de Materiales y Fluidos, CPS and I.C.M.A., 50015 Zaragoza, Spain*

(Received 3 February 1998)

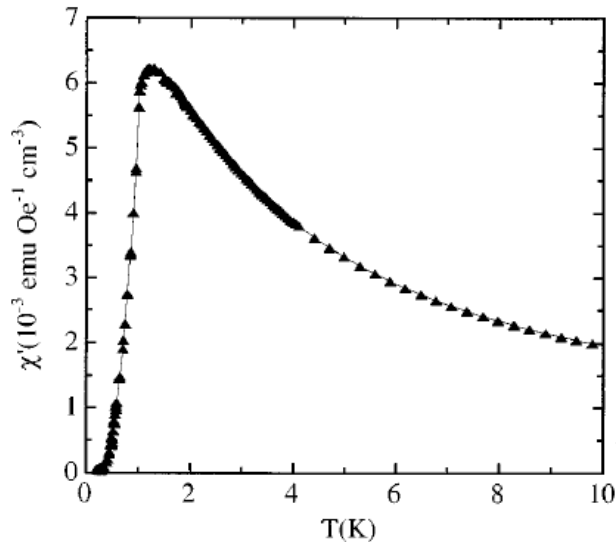


FIG. 1. Magnetic susceptibility of NdGaO<sub>3</sub> along [001].

used to measure the microwave frequency. The Nd content of the doped LaGaO<sub>3</sub> sample was determined by electron probe microanalysis to be  $(2.1 \pm 0.3) \times 10^{20}$  Nd<sup>3+</sup> ions/cm<sup>3</sup>.

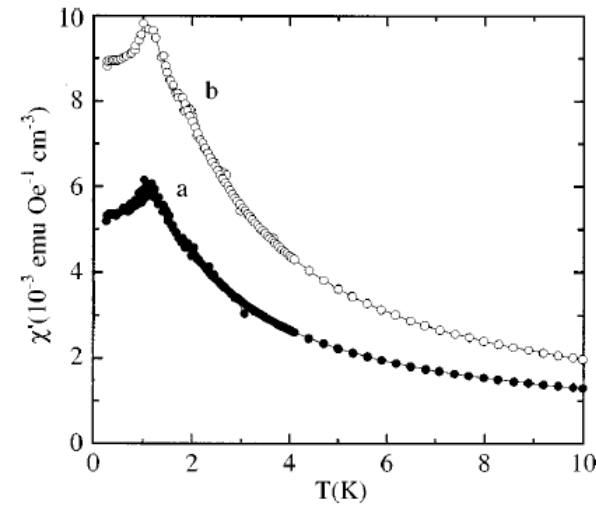


FIG. 2. Magnetic susceptibility of NdGaO<sub>3</sub> along [100] (a), and [010] (b).

TABLE II. Critical temperature,  $g$ -tensor components, and exchange parameters obtained from the analysis of the experimental data.

Expt.	$T_c$ (K)	$g_x$	$g_y$	$g_z$	$J_{\perp}/k$ (K)	$r$
$C_p$	$0.97 \pm 0.01$				$-0.70 \pm 0.01$	$-0.10 \pm 0.02$
$\chi_{\parallel}$				$2.73 \pm 0.02$	$-0.70 \pm 0.01$	$-0.10 \pm 0.02$
$\chi_{\perp, \max}$		$1.80 \pm 0.02$	$2.28 \pm 0.02$		$-0.86 \pm 0.05$	
$\chi_{\perp}(T=0)$		$1.84 \pm 0.02$	$2.41 \pm 0.02$			
EPR		$2.025 \pm 0.005$	$2.495 \pm 0.005$	$2.72 \pm 0.01$		

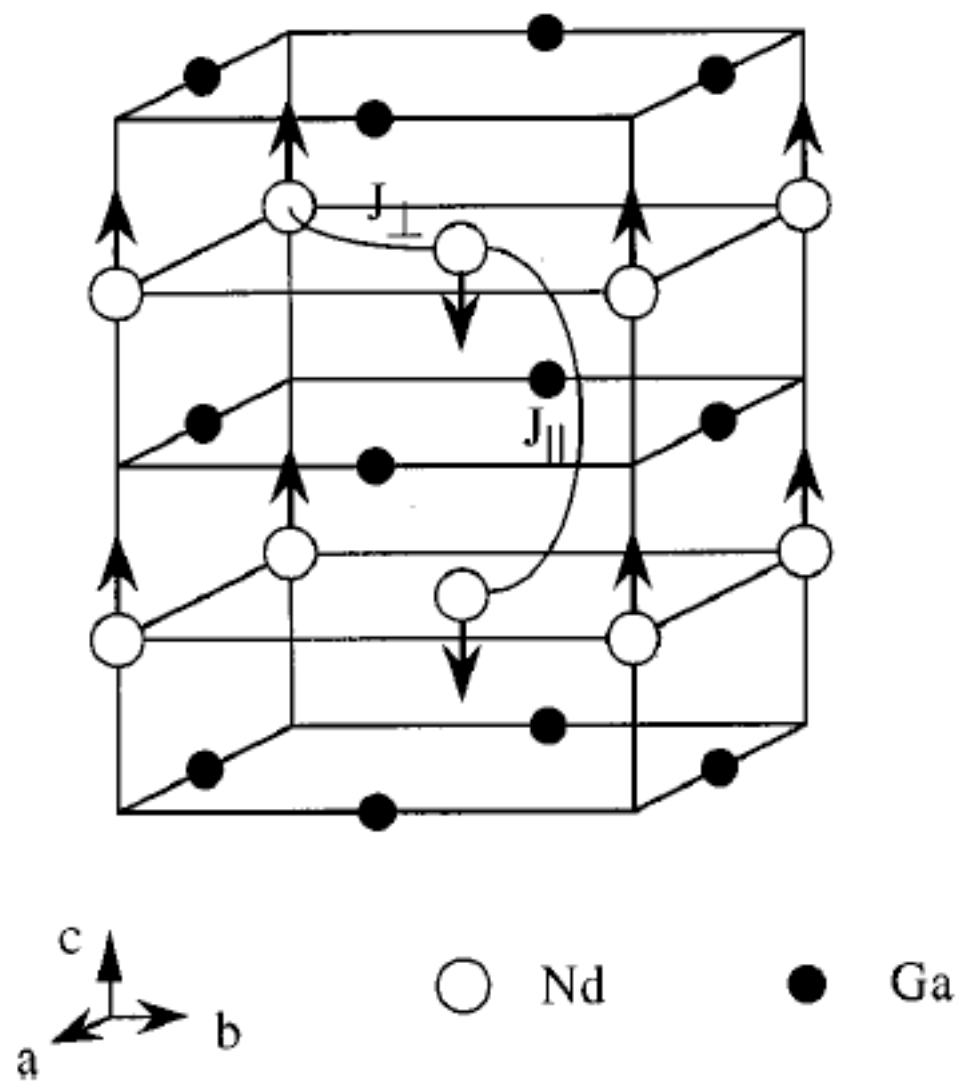


FIG. 3. Magnetic structure  $C_2$  of  $\text{NdGaO}_3$  (oxygen atoms are not depicted).

### Specific heat and magnetic interactions in NdCrO<sub>3</sub>

Fernando Bartolomé and Juan Bartolomé  
 ICMA, CSIC-Universidad de Zaragoza, 50009 Zaragoza, Spain

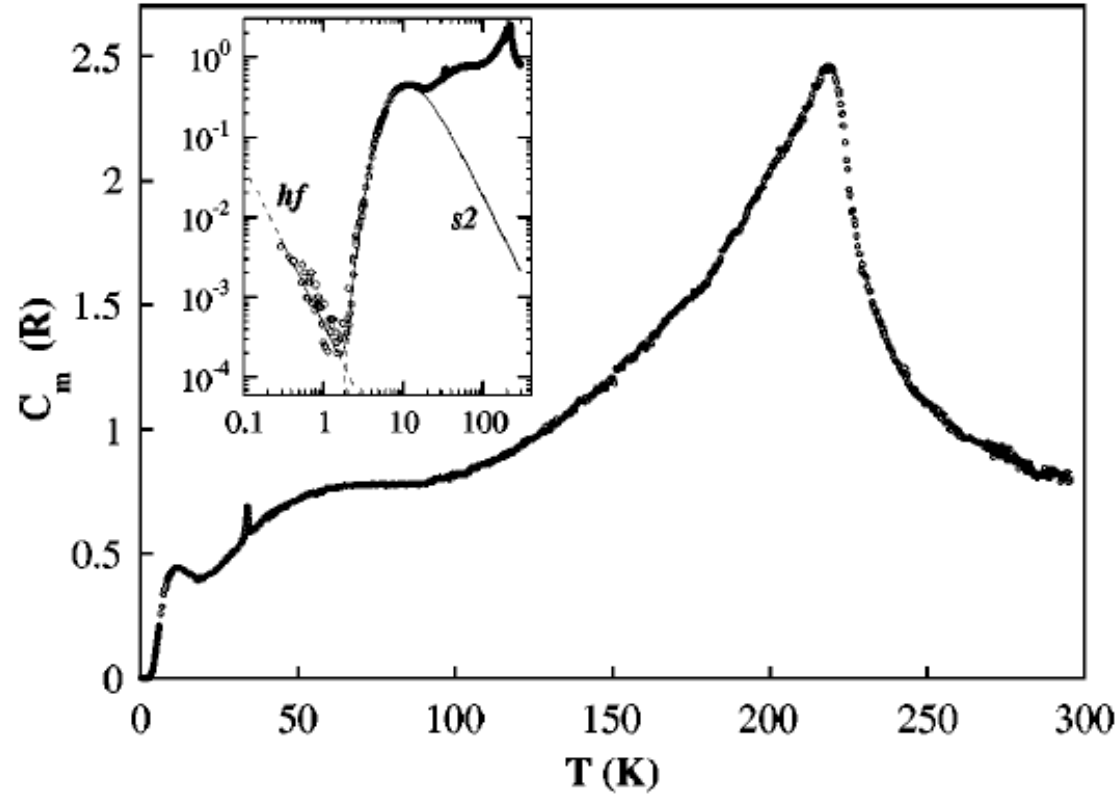


FIG. 2. Magnetic specific heat of NdCrO<sub>3</sub>,  $C_m$ . The inset shows the same data on a double-log scale. The fitted hyperfine (hf) and two-level Schottky ( $s_2$ ) contributions are also shown.

$$C_{hf}/R = \frac{\overline{\mu_{eff}^2} \cdot H_{hf}^2}{3k_B^2 T^2},$$

$$C_{sw}/R = 13.7 \left( \frac{k_B T}{12JS} \right)^3$$

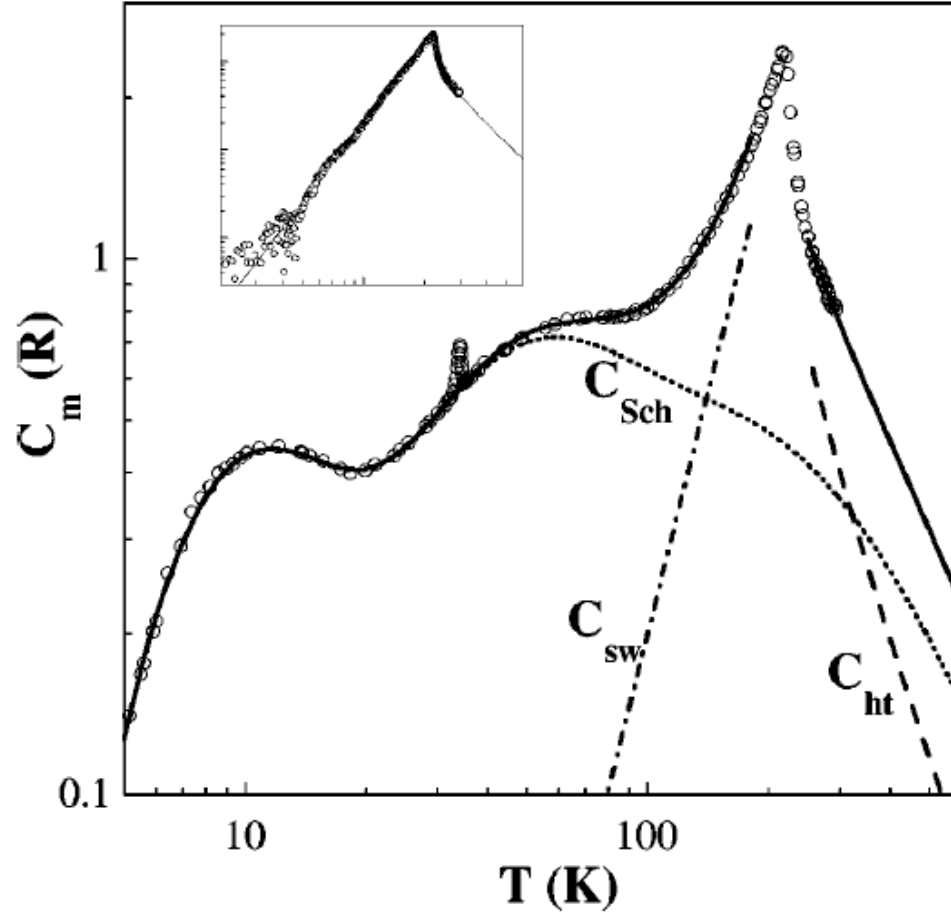


FIG. 5. Magnetic specific heat of  $\text{NdCrO}_3$  (open symbols) on a double-log scale. For the sake of clarity, only a part of the data is shown. The three separate contributions to the calculated  $C_m$  (solid line) are shown;  $\text{Nd } ^4I_{9/2}$  Schottky,  $C_{Sch}$  (dotted line), magnonic contribution of the Cr subsystem,  $C_{sw}$  (dash-dotted line), and s.c.  $S=3/2$ , isotropic Heisenberg high-temperature specific heat,  $C_{ht}$  (dashed line). The inset shows the data on a double-log scale, once  $C_{Sch}$  has been subtracted, isolating the Cr magnetic contributions (except for the spin reorientation transition peak at  $T=34$  K).

simple cubic,  $S=3/2$ , isotropic Heisenberg Hamiltonian,

$$C_{ht}/R = \frac{2z(S(S+1))^2}{3\theta^2} \left( 1 + \sum_{n=1}^5 \frac{c_n}{\theta^n} \right) \quad (3)$$

where  $z$  is the number of nearest neighbors (6 for the s.c. lattice),  $\theta = k_B T/J$  and  $c_n$  are the expansion coefficients, given in Ref. 29 up to  $n=5$ . The best fit of  $C_m$  above 250 K is shown in Fig. 5, yielding the result  $|J_{Cr}^{ht}|/k_B = 21.6(5)$  K.



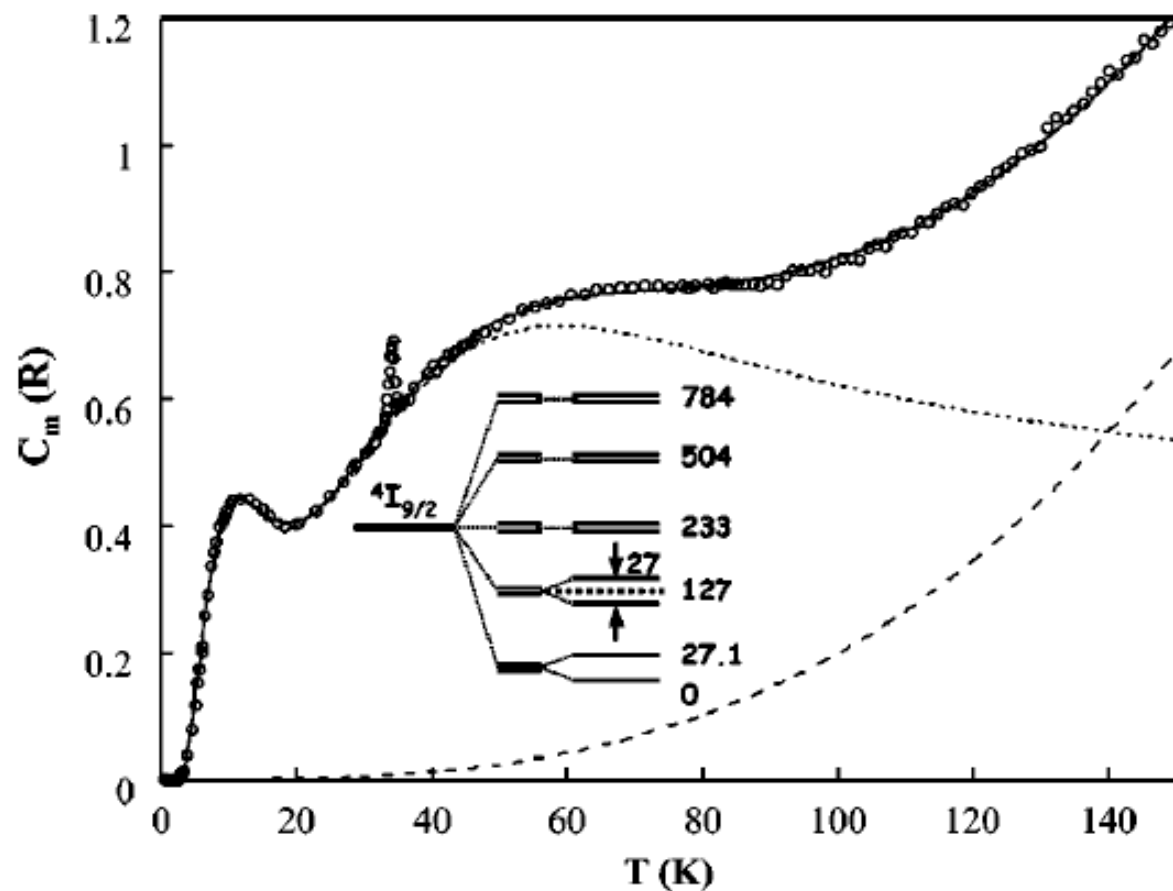


FIG. 4. Magnetic specific heat of  $\text{NdCrO}_3$  below 150 K (open symbols). The fitted curve (solid line) is the sum of the Schottky curve from  $\text{Nd } ^4I_{9/2}$  (dotted line) and the magnonic specific heat of the Cr subsystem (dashed line). The crystal-field energies derived from the fit is shown in the scheme. For the sake of clarity, only one half of the data is shown.

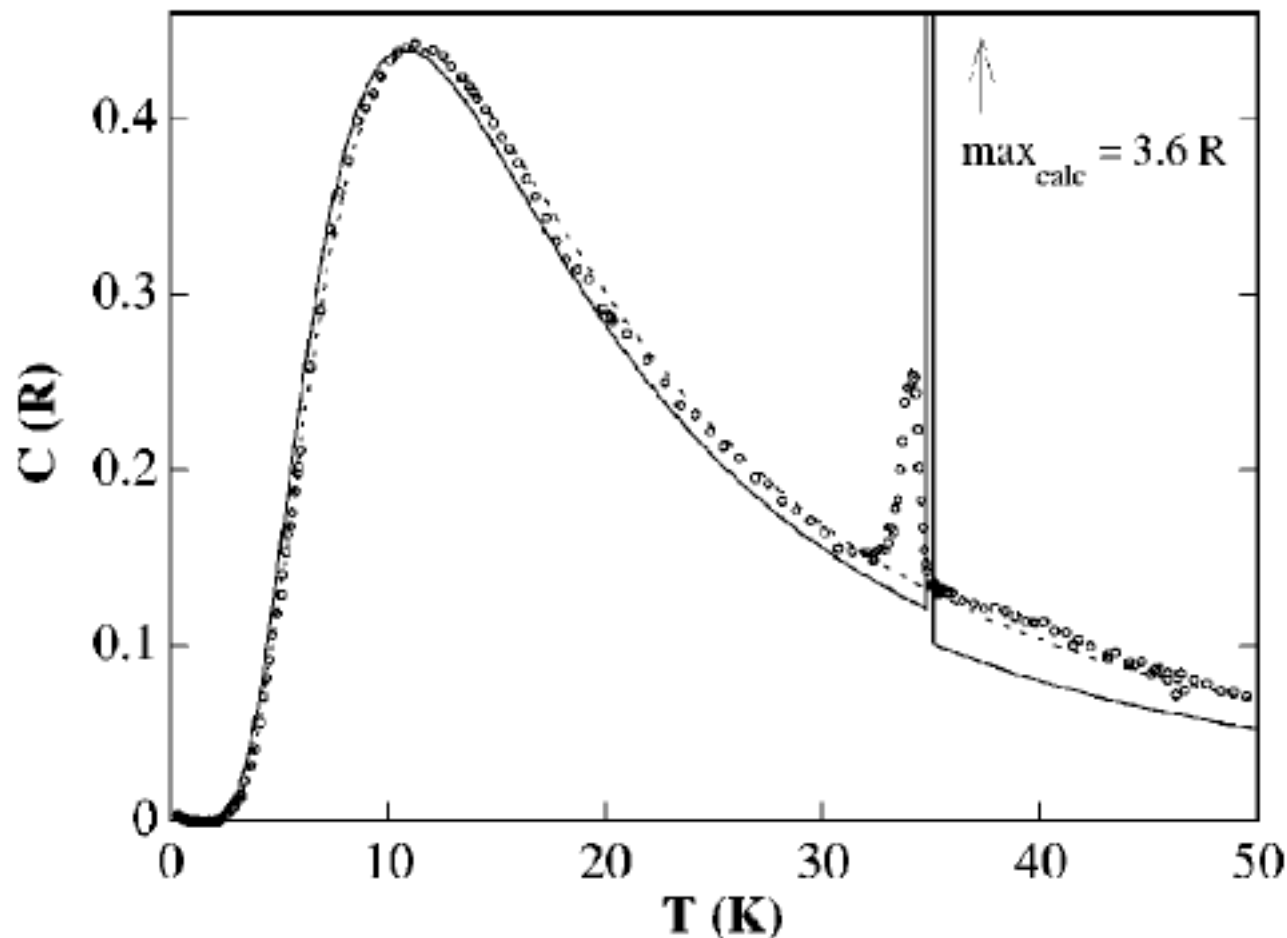


FIG. 9. Specific-heat Schottky contribution of the Nd ground doublet, compared to the Hornreich's prediction (solid line) presenting a discontinuity of  $0.02R$  at  $T_{SRT}$  and a sharp anomaly characteristic of a first-order transition. The theoretical curve obtained from our fit, with  $\Delta_g/k_B = 27.15$  K (dotted line), is also shown.

**Single-crystal neutron diffraction study of Nd magnetic ordering in NdFeO<sub>3</sub> at low temperature**

J. Bartolomé, E. Palacios, M. D. Kuz'min, and F. Bartolomé

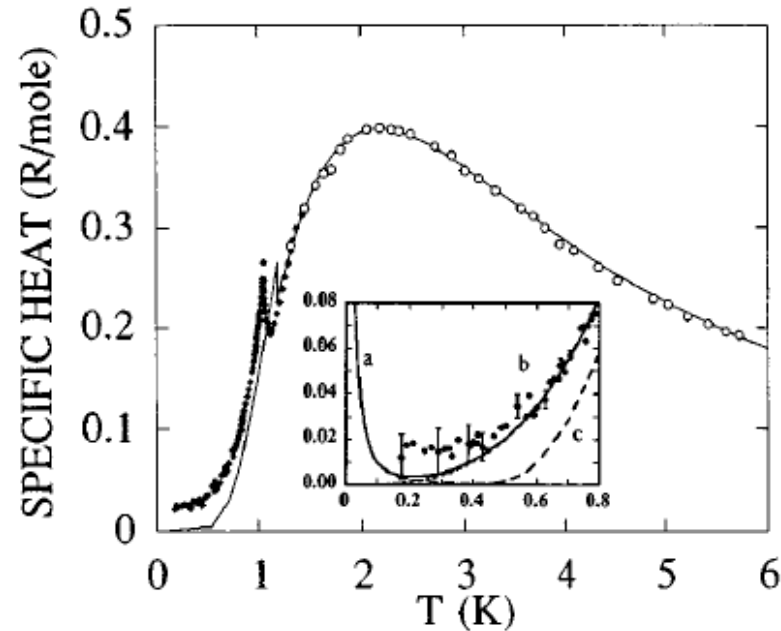
*Instituto de Ciencia de Materiales de Aragón, CSIC-Universidad de Zaragoza, 50009 Zaragoza, Spain*

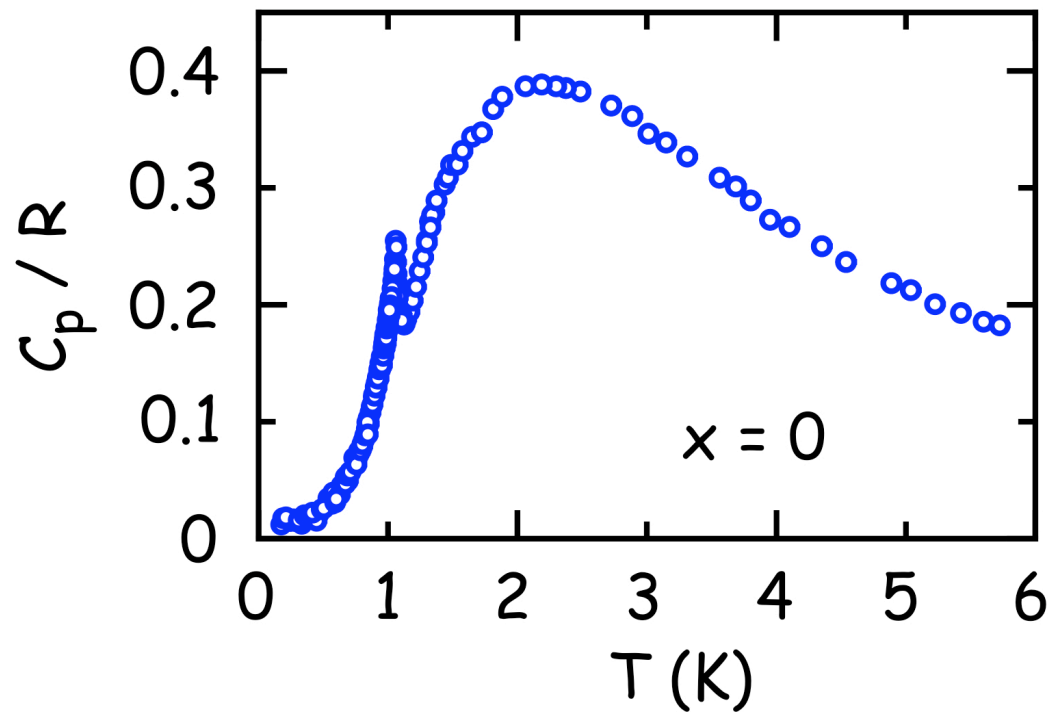
FIG. 5. Temperature dependence of the specific heat of NdFeO<sub>3</sub>:  $\blacklozenge$  experiment, Ref. 2;  $\circ$  experiment, Ref. 3; continuous curve—calculation, see the text. Inset;  $\bullet$  low-temperature data. (a) Hyperfine contribution calculated with  $H_{\text{hf}}=1$  MOe, (b) spin-wave contribution, (c) mean-field model calculation.







**x=0**



## Spin Hamiltonian for the Nd system

$$\mathcal{H} = -2 \theta_c \gamma \hat{\mathbf{g}}_x - 2 \theta_p \chi \hat{\mathbf{c}}_y + g_y \mu_B H_{\text{Fe-Nd}} \hat{\mathbf{c}}_y - 2 \theta_c \gamma^2 - 2 \theta_p \chi^2$$



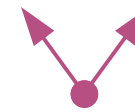
Nd-Nd exchange of the polarized component



Fe-Nd Zeeman term (eff. exchange field)



Self interaction terms



Nd-Nd exchange in cooperative mode

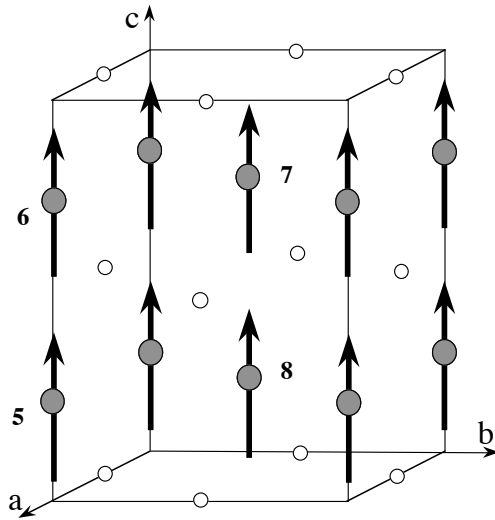
*where...*

$\gamma = -\frac{1}{2} \langle \hat{\mathbf{g}}_x \rangle$  and  $\chi = -\frac{1}{2} \langle \hat{\mathbf{c}}_y \rangle$  are mean field order parameters for the cooperative and induced modes

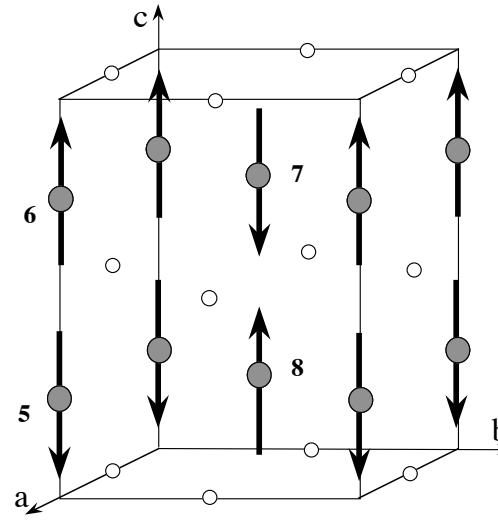
$\theta_c$  and  $\theta_p$  are the Nd-Nd exchange constants in cooperative and polarized modes



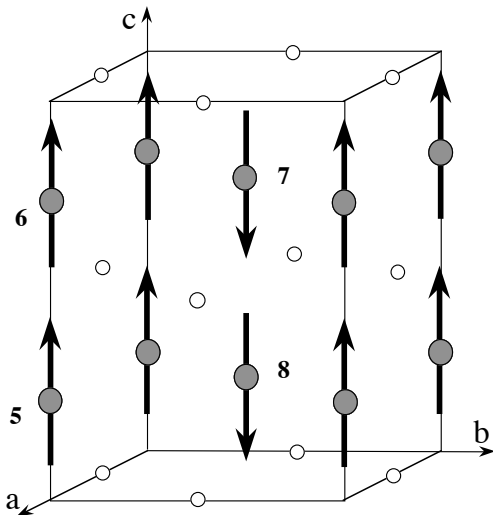
# Antiferromagnetic Bertaut's modes



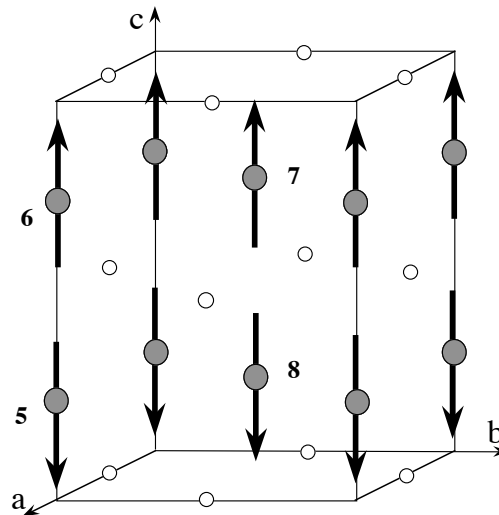
Modo  $f_z$



Modo  $g_z$



Modo  $c_z$



Modo  $a_z$

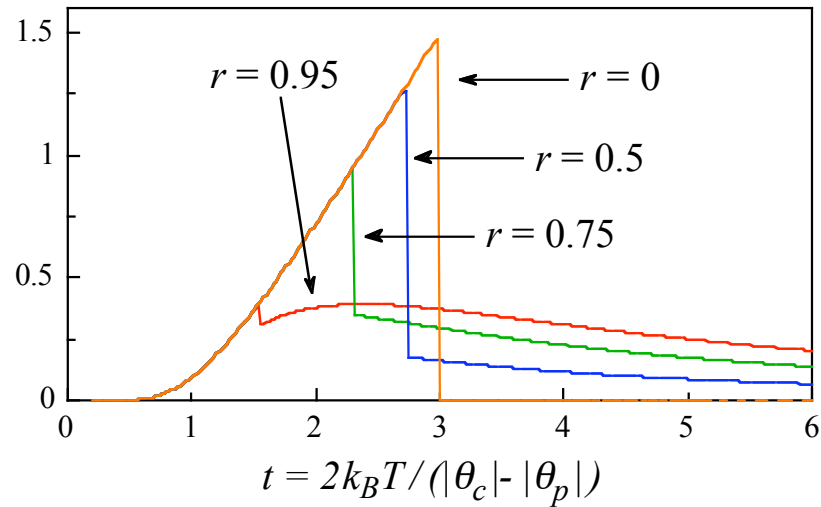
$$\hat{\mathbf{f}}_{M,R} = \hat{\mathbf{s}}_{1,5} + \hat{\mathbf{s}}_{2,6} + \hat{\mathbf{s}}_{3,7} + \hat{\mathbf{s}}_{4,8}$$

$$\hat{\mathbf{g}}_{M,R} = \hat{\mathbf{s}}_{1,5} - \hat{\mathbf{s}}_{2,6} + \hat{\mathbf{s}}_{3,7} - \hat{\mathbf{s}}_{4,8}$$

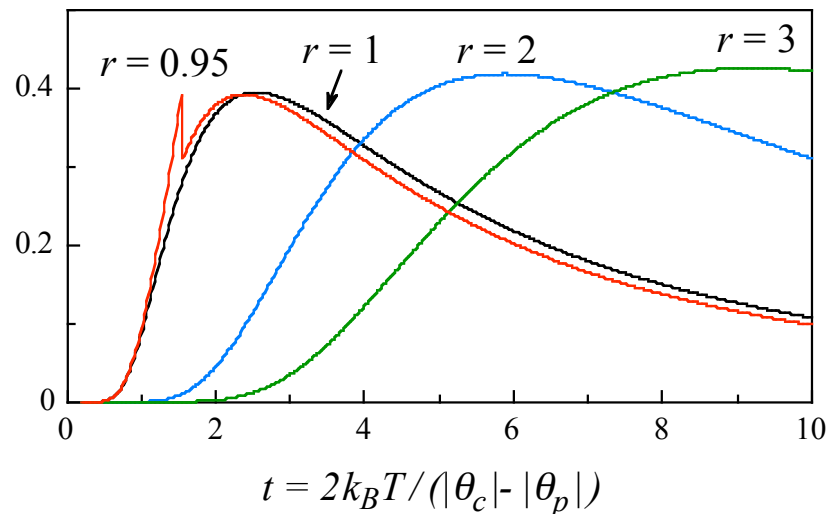
$$\hat{\mathbf{c}}_{M,R} = \hat{\mathbf{s}}_{1,5} + \hat{\mathbf{s}}_{2,6} - \hat{\mathbf{s}}_{3,7} - \hat{\mathbf{s}}_{4,8}$$

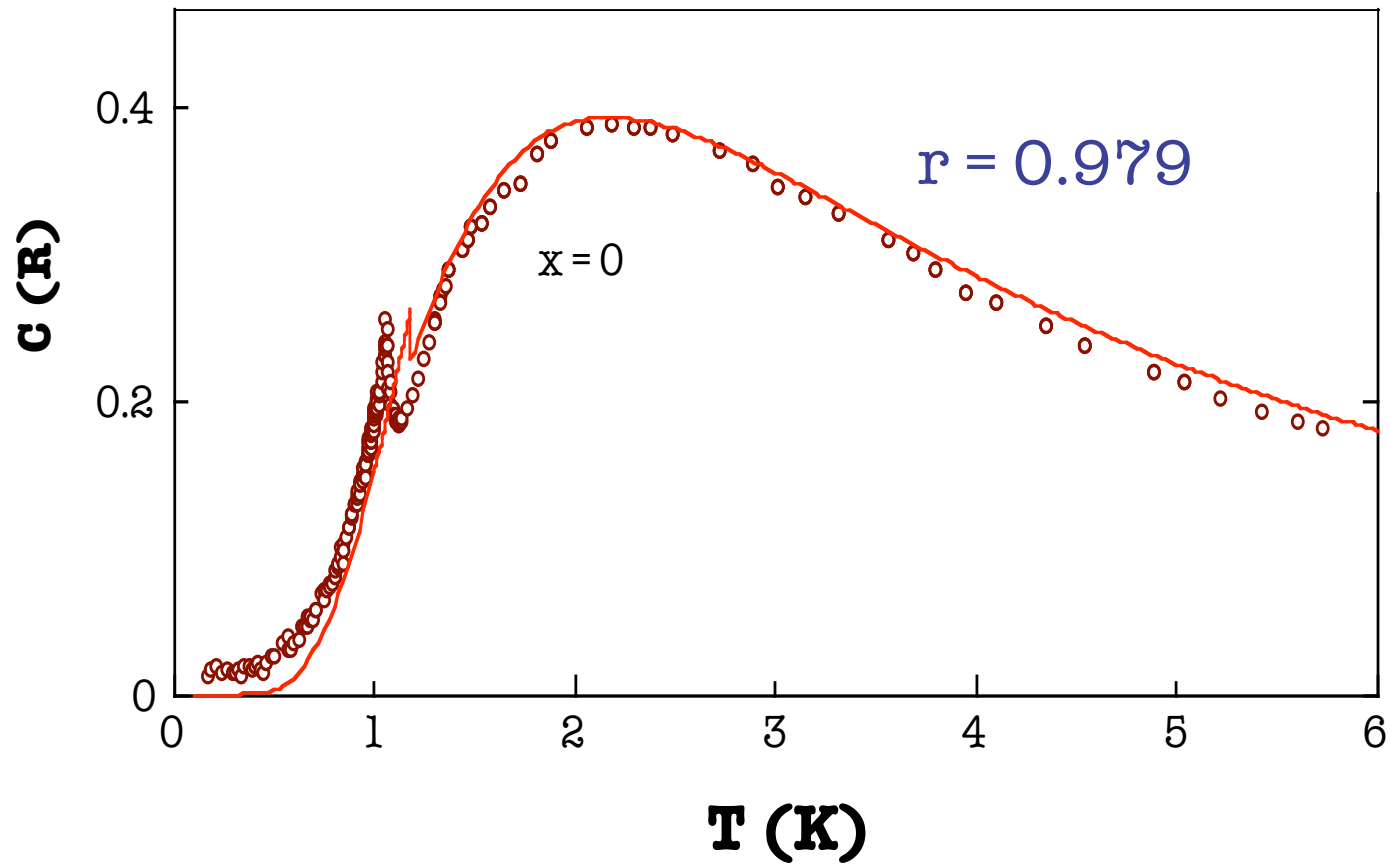
$$\hat{\mathbf{a}}_{M,R} = \hat{\mathbf{s}}_{1,5} - \hat{\mathbf{s}}_{2,6} - \hat{\mathbf{s}}_{3,7} + \hat{\mathbf{s}}_{4,8}$$

# Mean-field Model results

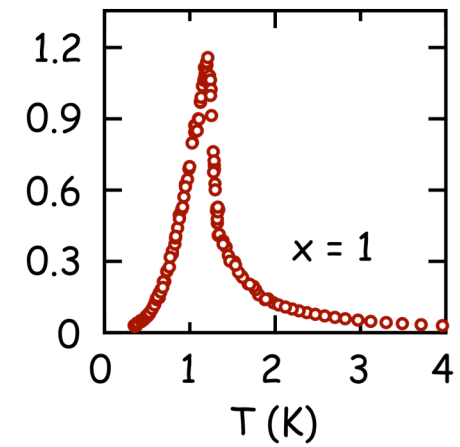
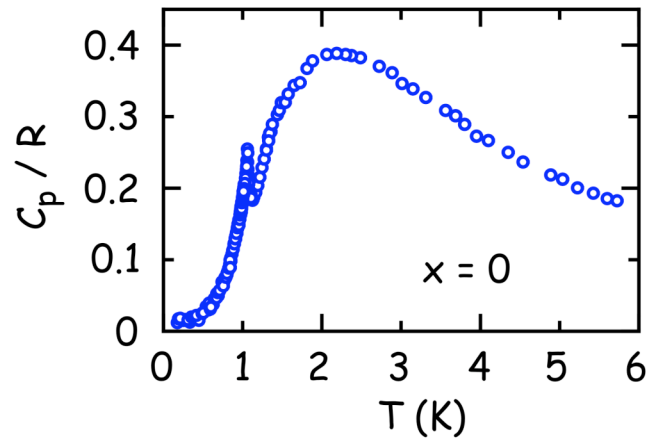


$$r = \frac{g_y \mu_B H_{Fe-Nd}}{2(|\theta_p| - |\theta_c|)}$$

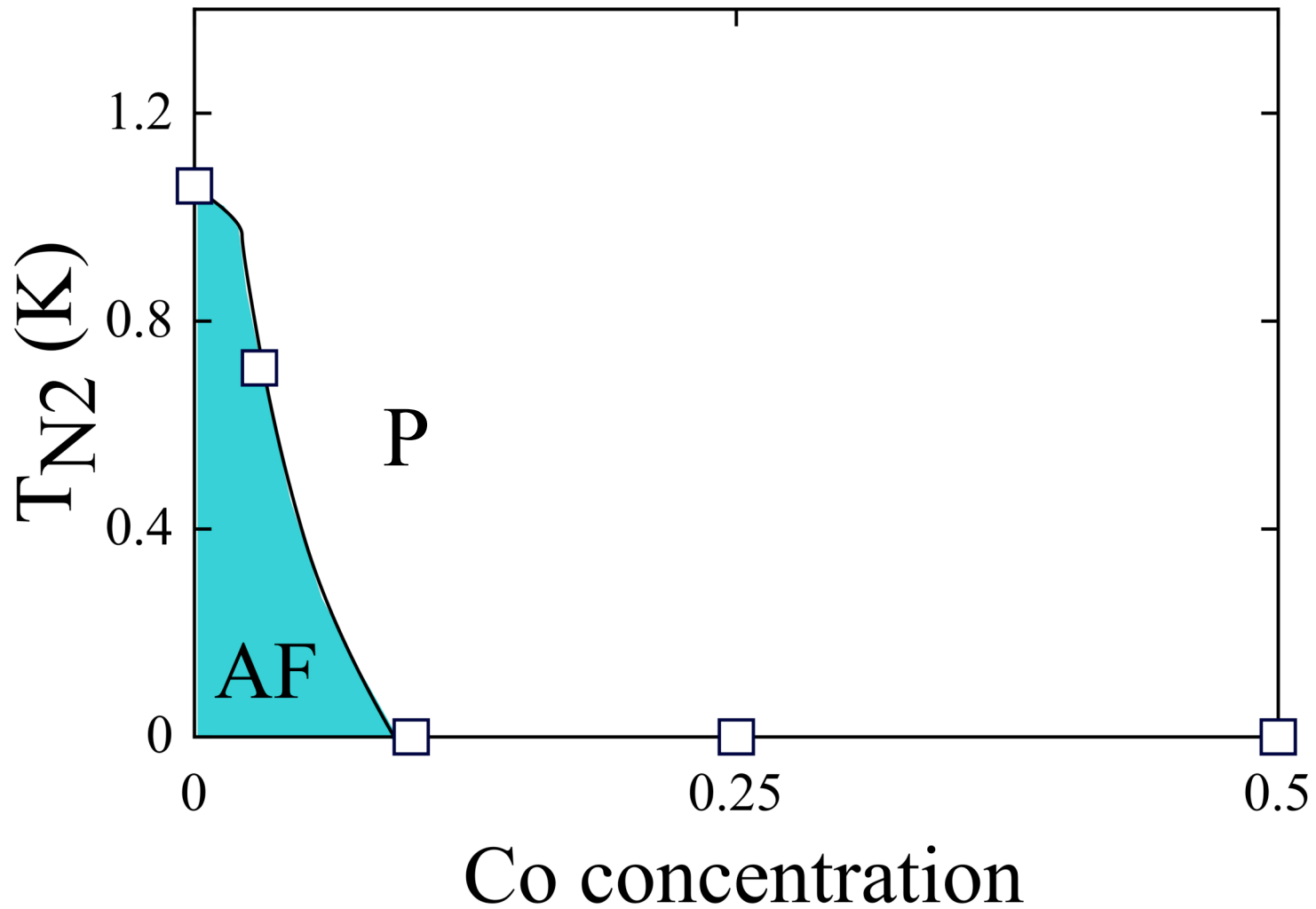




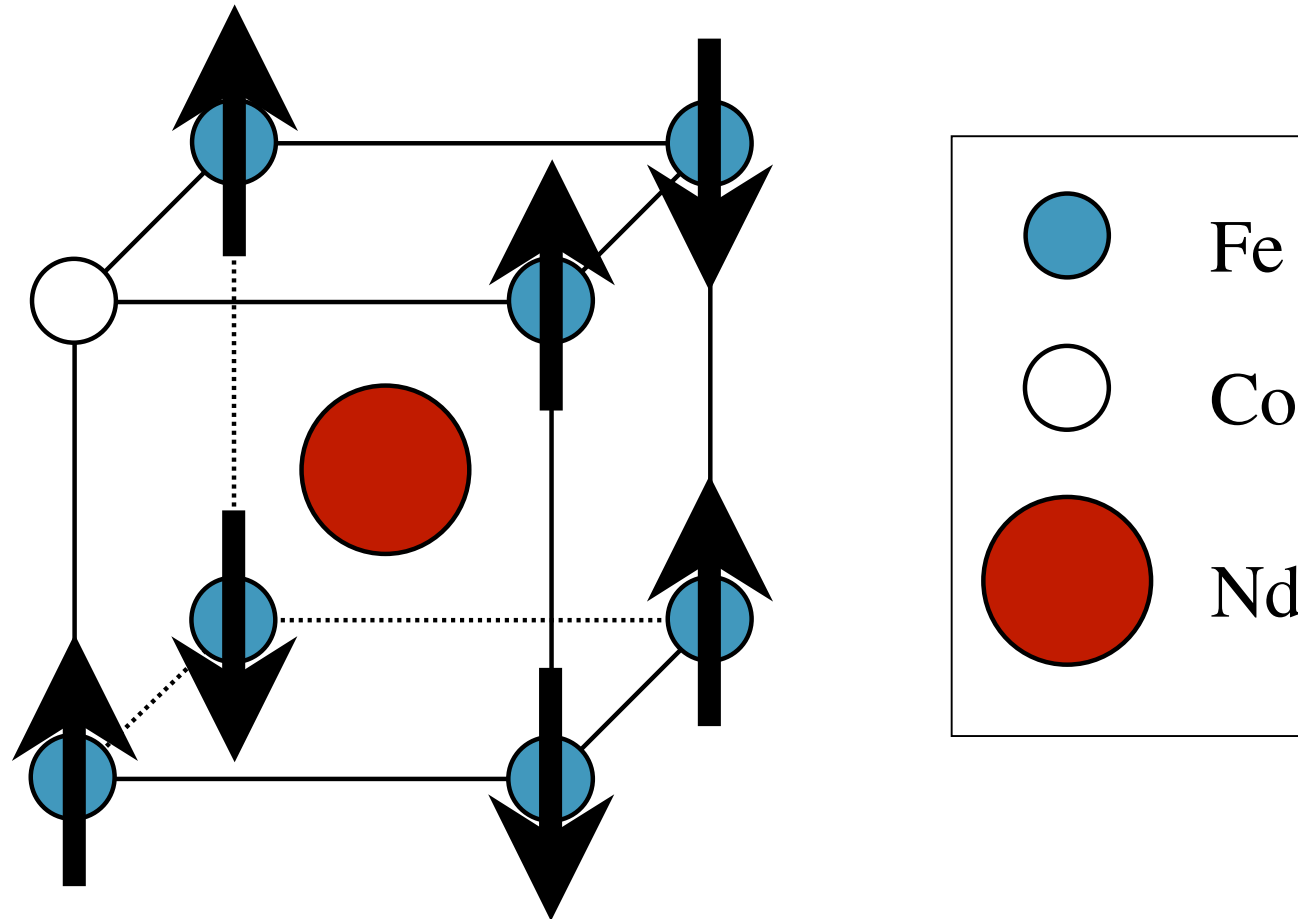
# Specific heat results



# Nd Phase diagram



# magnetic vacancies



## Spin Hamiltonian for the Nd system

$$\mathcal{H} = -2 \theta_c \gamma \hat{\mathbf{g}}_x - 2 \theta_p \chi \hat{\mathbf{c}}_y + g_y \mu_B \mathbf{H}_{\text{Fe-Nd}} \hat{\mathbf{c}}_y -$$

$$2 \theta_c \gamma^2 - 2 \theta_p \chi^2$$

$$H_{eff} = \frac{z-2}{z} H_{Fe-Nd} + \eta H_{ex} c_y$$

$$\mathcal{F} = \frac{1}{2} \theta_c \gamma^2 + \frac{1}{2} \theta_p \chi^2 + (1 - zx) T \ln \left[ 2 \cosh \left( \frac{\Delta}{2T} \right) \right] +$$

$$\frac{1}{2} \sum_{\eta=\pm 1} (zx) T \ln \left[ 2 \cosh \left( \frac{\Delta^\pm}{2T} \right) \right]$$

