THE MAGNETIC PHASE TRANSITION IN $KDy(MoO_4)_2$[1])

МАГНИТНЫЙ ФАЗОВЫЙ ПЕРЕХОД В $KDy(MoO_4)_2$

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The layered $KDy(MoO_4)_2$ shows an orthorombic crystallographic structure (space group D_{2h}^{14}) at room temperatures ($a = 1.82$ nm, $b = 0.795$ nm, $c = 0.507$ nm). It undergoes a crystallographic second-order phase transition of the Jahn—Teller type to an antiferrodistortive phase below 14 K. Above this temperature the Dy^{3+} ions have a low-lying doublet 35.7×10^{-23} J above the ground doublet state. When the substance is cooled through the transition temperature these doublets move symmetrically apart in energy to a low-temperature splitting of 55.6×10^{-23} J [1]. The phase transition in the complex magnetic ordered state was found at 1.1 K by magnetic susceptibility measurements [1]. The heat capacity measurements were performed in [1] from 3 K but their precise analysis was not made due to a large Schottky contribution and lattice contribution.

In this paper the results of the heat capacity measurements in the temperature range from 0.5 K to 6 K are presented. The single crystal sample (mass 1.2 g) was prepared by the flux method. The heat capacity was measured by means of the usual heat pulse method [2]. The heat capacity of the measured sample from 0.5 K to 6 K is shown in Fig. 1. The lambda type peak at (1.000 ± 0.005) K corresponds to the magnetic phase transition. The obtained value for T_c differs from $T_c = 1.1$ K mentioned in [1]. The total heat capacity C_T may be written as a sum of the lattice contribution C_L, the heat capacity caused by the crystal field splitting (Schottky anomaly) C_{SH} and the magnetic contribution C_M

$$C_T = C_L + C_{SH} + C_M. \tag{1}$$

C_{SH} was calculated for a two-level system with $\Delta E = 55.6 \times 10^{-23}$ J and was separated from the total heat capacity (dashed line in Fig. 1). Many of the models for the magnetic contribution have a T^{-2} dependence for the heat capacity in the high temperature limit and the lattice heat capacity follows the T^3 law in the low temperature limit. The rest of the heat capacity $(C_T - C_{SH})$ should obey the relationship

$$C_T - C_{SH} = sT^3 + bT^{-2} \tag{2}$$

in certain temperature range. To find this temperature range it is necessary to determine the linear interval on the $(C_T - C_{SH})T^2$ vs. T^5 plot. This region was found to extend from 2.14 K to 4.17 K. The parameters a, b were calculated by the least squares method as $a = (3.03 \pm 0.04)$ mJ/mol K^4 ($\Theta_D = (137.4 \pm 0.5)$) K was evaluated from a) and $b = (3.03 \pm 0.04)$ mJ K/mol (Fig. 2). For describing the magnetic heat capacity below 2.14 K the suitable low-dimensional magnetic model should be used. The deviation from the linear dependence above 4.17 K is probably due to the

[1]) Contribution presented at the 8th Conference on Magnetism, KOŠICE 29. 8.—2. 9. 1988

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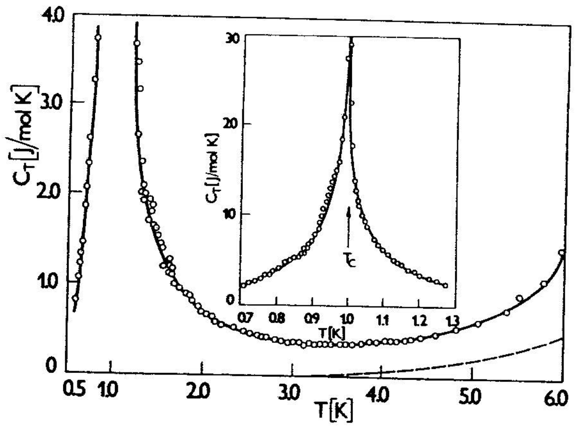

Fig. 1. Heat capacity of $KDy(MoO_4)_2$. The phase transition is indicated by an arow. The dashed line corresponds to a Schottky anomaly. The solid line is only a guide for eyes.

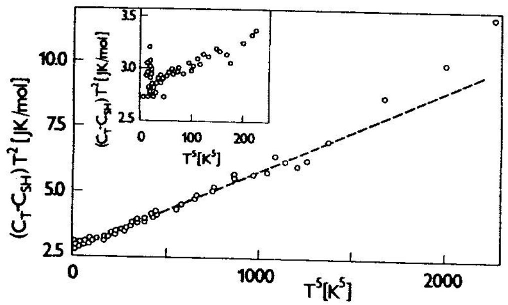

Fig. 2. Heat capacity data for $KDy(MoO_4)_2$, according to the relation (2). The insert shows a deviation from the linearity on the low temperature side.

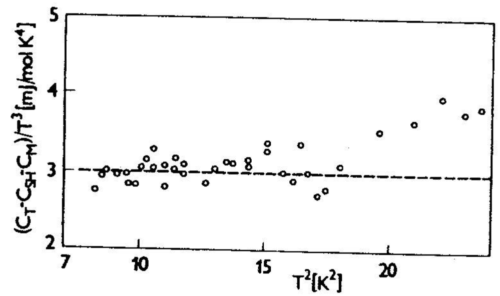

Fig. 3. Plot of the heat capacity data for $KDy(MoO_4)_2$ showing the deviation from the T^3 law on the high temperature side.

contribution of further terms of the temperature expansion of C_L. The contribution of the T^5 term to the C_L may be seen also on the $(C_T - C_{SH} - C_M)/T^3$ vs. T^2 plot (Fig. 3).

In conclusion, the magnetic phase transition into the ordered magnetic state was observed with $T_C = (1.000 \pm 0.005)$ K. For the magnetic part to the heat capacity in the T^{-2} limit the coefficient $b = (2712 \pm 20)$ mJ K/mol and for the lattice part in the T^3 limit the coefficient $a = (3.03 \pm 0.04)$ mJ/mol K^4 were calculated. The value of the Debye temperature was found as $\Theta_D = (137.4 \pm 0.5)$ K, considering four oscillating groups in $KDy(MoO_4)_2$.

We are grateful to Prof. A. I. Zvyagin and Dr. E. E. Anders for providing us with the $KDy(MoO_4)_2$ sample.

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Received November 1st, 1988
Accepted for publication February 17th, 1989