Magnetic order in Y_2BaCuO_5

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The compound Y_2BaCuO_5, which is the nonsuperconducting component of the high-T_c superconductor Y–Ba–Cu–O, has been found to possess magnetic order at 16.5 K.

The high-T_c superconductors Y–Ba–Cu–O generally have a green semiconducting phase Y_2BaCuO_5 in addition to the superconducting phase $YBa_2Cu_3O_{7-\delta}$.[1] Both of these compounds belong to the perovskite group and have common structural elements: CuO_5 pyramids. Since the green phase and the superconducting phase both have copper-oxygen chains, the data on the properties of the green phase may be useful in understanding the mechanism of superconductivity in high-T_c superconductors. In particular, in view of the discovery[2] of antiferromagnetic order in copper in the perovskite system $La_{2-x}Sr_xCuO_{4-\delta}$ (the high-T_c superconductors with lower values of T_c than that of $YBa_2Cu_3O_7$ belong to this system) with T_N which depend on x and δ, it is of interest to study magnetic order in systems which are related to high-T_c superconductors of the $YBa_2Cu_3O_{7-\delta}$ type.

We have detected magnetic order in the green phase Y_2BaCuO_5.

The optical spectra of the diffuse reflection of the powder samples $(Y_{0.99}Er_{0.01})_2BaCuO_5$ near the transitions $I_{15/2} - {}^4I_{13/2,11/2}$, in the ER^{3+} ion were studied experimentally. Figure 1 shows the low-temperature spectrum of ${}^4I_{15/2} - {}^4I_{13/2.}$ The shape of the spectrum suggests that there are two nonequivalent but only slightly different in the nearest neighborhood C_3 symmetry positions for yttrium

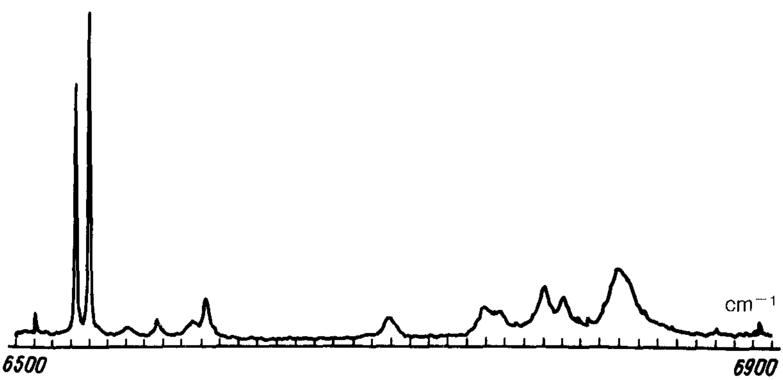

FIG. 1. Absorption in Y_2BaCuO_5 near the ${}^4I_{15/2}$–${}^4I_{13/2}$ (Er^{3+}) transition. Er (1%), $T = 20$ K.

(erbium) in Y_2BaCuO_5 (Ref. 1). The $^4I_{13/2}$ level for each center is split into a maximum number of sublevels without a magnetic field: Kramers doublets. Figure 2a is a plot of the temperature transformation of the spectrum near the narrowest low-frequency lines of the transition in the nonequivalent Er^{3+} centers. The temperature behavior of the positions and intensities of the components of the left doublet suggests that the splitting is associated with the appearance of a local magnetic field, rather than with the appearance of new nonequivalent positions for a rare-earth ion because of the change in the structure of the crystal as a result of a change in temperature.

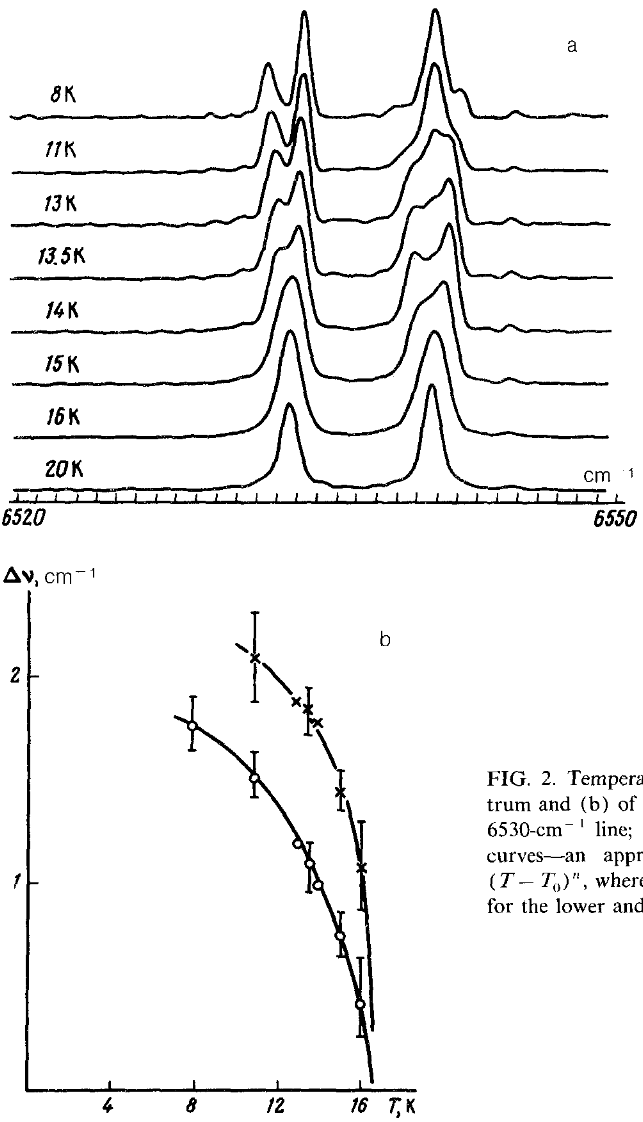

FIG. 2. Temperature dependences (a) of the spectrum and (b) of the line splitting. Open circles—the 6530-cm^{-1} line; crosses—the 6540-cm^{-1} line. Solid curves—an approximation using the dependence $(T-T_0)^n$, where $T_0 = 16.5$ K, and $n = 1/2$ and $1/3$ for the lower and upper curves, respectively.

Upon lowering the temperature the right doublet decreases in intensity, giving rise to the appearance and intensification of the nonshifted line.

An analysis of the temperature dependence of the splitting and intensities of the $^4I_{15/2}$–$^4I_{13/2,11/2}$ transitions (Er^{3+}) gives a magnetic-ordering temperature of 16.5 K and a 3.8-cm^{-1} ground-state splitting of Er^{3+} at 8 K for one center and 5.9 cm^{-1} for the other center. Estimating the values of the g-factor to be $g = 5$–10 in the ground state, we estimate the local field of the Er^{3+} ions to be $H = 8$–25 kOe.

The complex nature of the splitting of the right line (Fig. 2a) may stem from the spin-flip transition and thus from the existence of domains of various phases. The left line does not sense this transition, since the field of the corresponding center changes its direction in the plane in which the g-factor changes only slightly: the local axes of the two centers run in mutually perpendicular directions.[1]

The nature of magnetic order cannot be determined from optical data. An anomaly in the magnetic susceptibility at 13 K showed that the spin order of Cu^{2+} in a compound with a similar structure $Y_2Cu_2O_5$ is of an antiferromagnetic nature.[3]

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[1)] The observable line splitting (Fig. 2) corresponds to the difference in the splitting of the ground level and the excited level of the transition.

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[2] Y. J. Uemura, W. J. Kossler, X. H. Yu *et al.*, Phys. Rev. Lett. **59**, 1045 (1987).
[3] R. Troc, Z. Bucowski, R. Horin, and J. Klamut, Phys. Lett. **A125**, 222 (1987).

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