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Identification of the high-temperature superconducting phase in the Y-Ba-Cu-O system as the perovskite $YBa_2Cu_3O_{7\pm\delta}$

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Abstract. The oxide responsible for high-temperature superconductivity (onset ~ 100 K, zero resistance above liquid N_2 temperature) is found to be $YBa_2Cu_3O_{7\pm\delta}$.

Keywords. High-temperature superconductivity; $YBa_2Cu_3O_7$

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The discovery of superconducting oxides of the Y-Ba-Cu-O system, exhibiting zero resistance above the liquid nitrogen temperature (Wu *et al* 1987; Ganguly *et al* 1987), has received worldwide attention. The oxide compositions which have shown this behaviour seem to be complex and biphasic. The $Y_{1.2}Ba_{0.8}CuO_4$ composition of Wu *et al* (1987), based on the analogy with $La_{2-x}Ba_xCuO_4$ possessing the K_2NiF_4 structure (Chu *et al* 1987; Rao and Ganguly 1987), consisted of a green and a black oxide. We suspect that the green oxide was Y_2BaCuO_5 which is an insulator. We did not prepare Y-Ba-Cu oxides with compositions related to those of K_2NiF_4 structure since Y_2CuO_4 itself is not formed in this structure. Instead, we made Y-Ba-Cu oxides analogous to $La_3Ba_3Cu_6O_{14}$ (Er-Rakho *et al* 1981) which is an oxygen-deficient perovskite possessing a

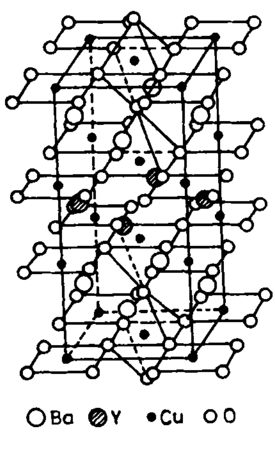

Figure 1. Proposed structure of $Y_2Ba_4Cu_6O_{14\pm\delta}$ analogous to $La_3Ba_3Cu_6O_{14}$ (following Er-Rakho *et al* 1981). A_1 and A_2 sites are shown. Y occupies A_2 sites preferentially.

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tetragonal structure with $a = a_p 2^{1/2}$ and $c = 3a_p$; the oxygen vacancies are ordered with three different copper sites. This as well as the analogous yttrium oxides are black and the a_p parameter decreases with the introduction of the smaller Y ion. Along the c-axis, the sequence is $|Cu_2O_4 - A_2O\square - Cu_2O_4 - A_2\square_2 - Cu_2O_4 - A_2O\square|_\infty$. The A cations with 8-coordination (A_1) and with 10-coordination (A_2) are occupied by Y (or La) and Ba ions respectively. This structure retains some features of the K_2NiF_4 structure in the sense that copper ions with essentially square-planar coordination do not

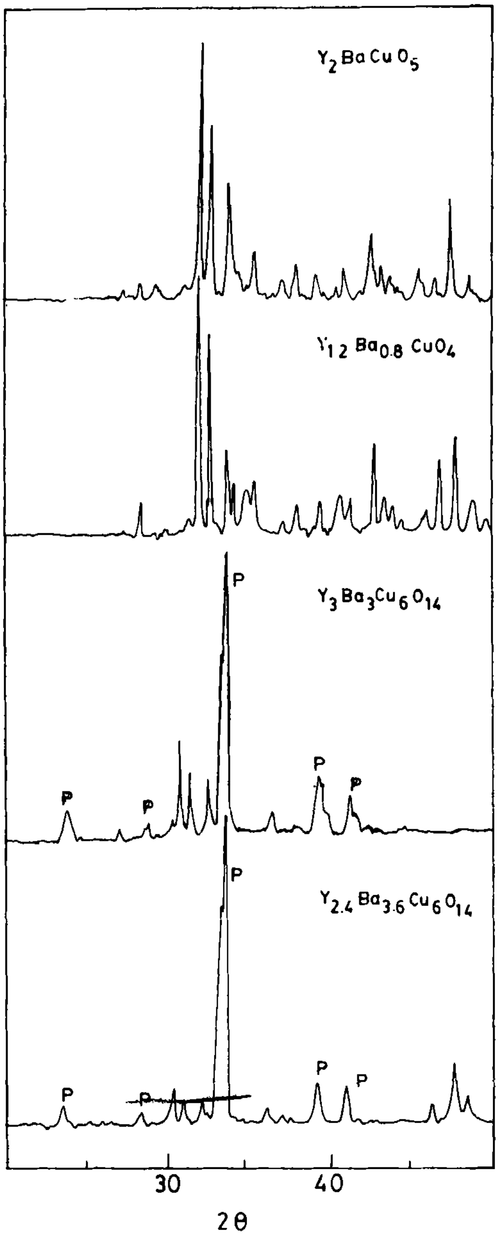

Figure 2. X-ray powder patterns of $Y_{3-x}Ba_{3+x}Cu_6O_{14}$, Y_2BaCuO_5 and $Y_{1.2}Ba_{0.8}CuO_4$.

interact along the c-axis over long distances. If Y occupies only A_2 sites, the composition will be $Y_2Ba_4Cu_6O_{14}$ (figure 1).

We have examined superconductivity of several oxides of the general formula $Y_{3-x}Ba_{3+x}Cu_6O_{14}$ and find some of them to be superconducting well above the liquid nitrogen temperature (Ganguly *et al* 1987; also unpublished results from this laboratory). Almost all the compositions are however biphasic. We have carried out an x-ray study of these oxides to establish the identity of the oxide phase responsible for high-temperature superconductivity. In figure 2, we show typical x-ray powder patterns of these oxides along with those of Y_2BaCuO_5 (green insulator) and $Y_{1.2}Ba_{0.8}CuO_5$ (composition of Wu *et al* 1987). We readily see that the last oxide has predominant features of Y_2BaCuO_5 and some weaker features of the perovskite; $Y_{3-x}Ba_{3+x}Cu_6O_{14}$ compositions, however, show the perovskite features (see intense peak marked P in figure 2). Prominently, features of Y_2BaCuO_5 are much weaker here. Based on this x-ray study, we find that the composition of the "pure" perovskite phase is likely to be close to $Y_2Ba_4Cu_6O_{14}$ or $YBa_2Cu_3O_7$. We have prepared this oxide composition by heating the component oxides in air at 1170 K and find it to be a monophasic perovskite. The perovskite phase in $Y_{3-x}Ba_{3+x}Cu_6O_{14}$ seems to be slightly less distorted compared to the pure $YBa_2Cu_3O_7$ phase; this probably arises from changes in oxygen stoichiometry. The exact composition of the high T_c oxide phase may therefore be written as $YBa_2Cu_3O_{7\pm\delta}$. This oxide heated in oxygen does indeed exhibit high-temperature superconductivity with zero resistance above liquid N_2 temperature.

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