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Structure of $Er_2Ba_2Cu_{1+x}Pt_{1-x}O_8$ ($x = 0{\cdot}1$)

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Abstract. $Er_2Ba_2Cu_{1+x}Pt_{1-x}O_8$ ($x = 0{\cdot}1$), $M_r = 982{\cdot}7$, orthorhombic, *Pcmn*, $a = 10{\cdot}273$ (2), $b = 5{\cdot}653$ (1), $c = 13{\cdot}137$ (3) Å, $V = 762{\cdot}9$ Å^3, $Z = 4$, $D_x = 8{\cdot}56$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71073$ Å, $\mu = 51{\cdot}9$ mm^{-1}, $F(000) = 414$, room temperature, final $R = 0{\cdot}060$ for 1128 [$|F_o| > 3\sigma(F_o)$] unique reflections. The crystal contains double zigzag chains composed of Cu, O and Pt ions running parallel to the *b* axis. The Cu ion has distorted square-pyramidal geometry and the Pt ion distorted octahedral geometry.

Introduction. Recently, structural studies have been reported on high-T_c superconductors: $La_{1.85}Sr_{0.15}CuO_4$ (Cava, Santoro, Johnson & Rhodes, 1987) and $YBa_2Cu_3O_7$ (Beno, Soderholm, Capone, Hinks, Jorgensen, Grace, Schuller, Segre & Zhang, 1987; Izumi, Asano, Ishigaki, Takayama-Muromachi, Uchida, Watanabe & Nichikawa, 1987).

During synthesis of $ErBa_2Cu_3O_7$ single crystals, the title compound was obtained, in which a large diamagnetic signal was reproducibly observed below 80–90 K (Shishido, Fukuda, Toyota, Ukei & Sasaki, 1987). The crystal structure of this new compound is described here.

Experimental. The crystal was prepared as described elsewhere (Shishido *et al.*, 1987). Crystal size 0·43 × 0·09 × 0·09 mm; Rigaku AFC-6A four-circle diffractometer, graphite-monochromated Mo $K\alpha$ radiation; lattice parameters from 12 reflections ($60 < 2\theta < 63°$); ω–2θ scan mode, scan speed 4° min^{-1} (ω); data collection up to $2\theta = 60°$; three standard reflections with no significant intensity variation; 4657 reflections measured (h: $-14 \to 14$, k: $-7 \to 7$, l: $0 \to 18$), of which 1128 unique reflections with $F_o > 3\sigma(F_o)$ are considered observed, $R_{\text{int}} = 0{\cdot}034$; absorption correction ($15{\cdot}07 < A^* < 80{\cdot}57$), correction for Lorentz and polarization effects.

From the possible space groups, *Pcmn* and $Pc2_1n$, *Pcmn* is adopted from the statistical distribution of the observed intensities. *Pcmn* proved to be the correct choice also in later stages of structure determination.

The structure was solved by direct methods, using a version of *MULTAN* (Main, Woolfson & Germain, 1971) to locate Pt, Er and Ba ions.

Difference Fourier maps revealed the Cu and O atom positions. For the population parameter *x* of Cu atoms at the Pt position, 0·1 was used from a consideration of the results of chemical analysis and the *R* value. Refinement by full-matrix least squares on $|F|$ of positional and anisotropic thermal parameters for all atoms converged to a final $R = 0{\cdot}060$, $wR = 0{\cdot}079$ [$w = 1/\sigma^2(F)$] and $(\Delta/\sigma)_{\max} = 0{\cdot}23$ in the last cycle. The final difference Fourier map shows maximum and minimum heights of 4·6 and −7·7 e Å^{-3}. The value of *g* for the isotropic secondary extinction (Zachariasen, 1967) is $4{\cdot}6\ (1) \times 10^{-5}$.

All calculations were carried out using the *UNICS* III program system (Sakurai & Kobayashi, 1979) and full-matrix least-squares program *RADIEL* (Coppens, Guru Row, Leung, Stevens, Becker & Yang, 1979). Atomic scattering factors for the O^{2-} ion were taken from Tokonami (1965), and those for other ions from *International Tables for X-ray Crystallography* (1974).

Discussion. Final atomic coordinates and selected interatomic distances and angles are presented in Tables 1 and 2.* The projection of the structure along the *b* axis is shown in Fig. 1. As shown in Fig. 2, the crystal is built up from double zigzag chains composed of Cu, O and Pt ions running parallel to the *b* axis.

Towards the end of the crystal structure analysis, the authors were informed of a structural study on $Ba_3A_2PtCu_2O_{10}$ (A=Y or Ho) (Geiser, Porter, Wang,

Table 1. *Atomic fractional coordinates and equivalent isotropic thermal parameters* (Å^2) (*Hamilton*, 1959)

$$B_{\text{eq}} = \tfrac{4}{3}\textstyle\sum_i\sum_j B_{ij}a_ia_j.$$

	x	y	z	B_{eq}
Pt	0·5331 (2)	0·25	0·3062 (1)	0·39
Er(1)	0·8132 (2)	0·25	0·3580 (1)	0·70
Er(2)	0·9848 (2)	0·25	0·5823 (1)	0·71
Ba(1)	0·3139 (3)	0·25	0·7936 (2)	0·94
Ba(2)	0·5921 (3)	0·25	0·5774 (2)	0·97
Cu	0·2679 (5)	0·25	0·5394 (4)	0·92
O(1)	0·444 (2)	0·009 (4)	0·217 (1)	1·23
O(2)	0·638 (2)	0·005 (4)	0·385 (1)	1·26
O(3)	0·864 (2)	−0·006 (5)	0·493 (1)	1·02
O(4)	0·390 (3)	0·25	0·411 (2)	1·18
O(5)	0·686 (3)	0·25	0·206 (2)	0·92

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44800 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Allen & Williams, 1987). The structures of the title compound and $Ba_3A_2PtCu_2O_{10}$ do not conform to any of the simple prototype structures or a superstructure thereof. They have similar Cu and Pt coordination geometry: the Cu ion possesses distorted square-pyramidal geometry and the Pt coordination is a distorted octahedron. Nevertheless, they are very different from each other in structure in spite of similar synthesis conditions: the crystal structure of the title compound is columnar, whereas that of $Ba_3A_2PtCu_2O_{10}$ is not.

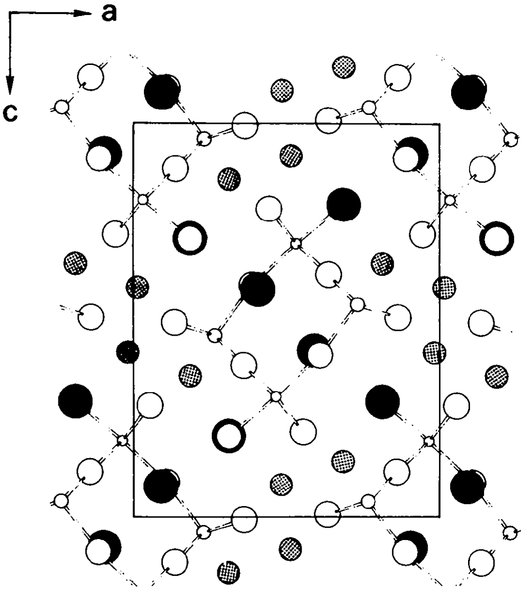

Fig. 1. Projection of the structure along the *b* axis. Atom key: open circles O (large), Cu (medium), Pt (small), dotted circles Er filled circles Ba.

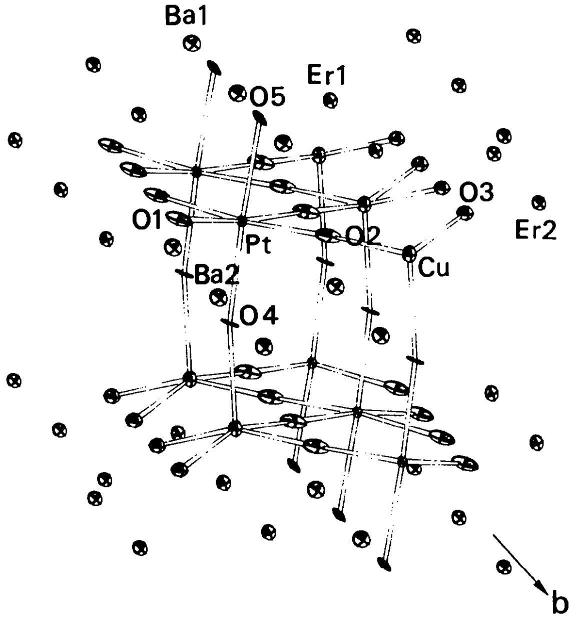

Fig. 2. An *ORTEP* drawing (Johnson, 1965) of a double zigzag chain of Cu, O and Pt ions and the surrounding Er and Ba ions.

Table 2. *Interatomic distances* (Å) *and angles* (°)

Pt—O(1)	2·02 (2)	Pt—O(2)	2·04 (2)
Pt—O(4)	2·02 (3)	Pt—O(5)	2·05 (3)
Cu—O(2^{i})	2·00 (2)	Cu—O(3^{i})	1·98 (2)
Cu—O(4)	2·10 (3)	Er(1)—O(2)	2·30 (2)
Er(1)—O(3)	2·35 (2)	Er(1)—O(5)	2·39 (3)
Er(1)—O(1^{vi})	2·22 (2)	Er(2)—O(3)	2·24 (2)
Er(2)—O(1^{vii})	2·35 (2)	Er(2)—O(5^{vii})	2·39 (3)
Er(2)—O(3^{viii})	2·30 (2)	Ba(1)—Cu	3·372 (5)
Ba(1)—O(1^{i})	2·89 (2)	Ba(1)—O(2^{i})	2·79 (2)
Ba(1)—O(5^{ii})	2·827 (1)	Ba(1)—O(1^{iv})	3·14 (2)
Ba(1)—O(3^{v})	3·16 (2)	Ba(1)—O(4^{iv})	2·60 (3)
Ba(2)—O(2)	2·92 (2)	Ba(2)—O(3)	3·33 (2)
Ba(2)—O(1^{i})	3·10 (2)	Ba(2)—O(2^{i})	2·82 (2)
Ba(2)—O(4)	3·01 (3)	Ba(2)—O(4^{ii})	2·836 (2)
Ba(2)—O(5^{vii})	2·83 (3)		
O(1)—Pt—O(2)	94·4 (8)	O(1)—Pt—O(4)	93·8 (8)
O(1)—Pt—O(5)	88·5 (8)	O(1)—Pt—O(1^{iii})	84·9 (8)
O(2)—Pt—O(4)	92·3 (8)	O(2)—Pt—O(5)	85·4 (8)
O(2)—Pt—O(2^{iii})	85·7 (8)	O(4)—Pt—O(1^{iii})	93·8 (8)
O(4)—Pt—O(2^{iii})	92·3 (8)	O(5)—Pt—O(1^{iii})	88·5 (8)
O(5)—Pt—O(2^{iii})	85·4 (8)	O(2^{i})—Cu—O(3^{i})	86·4 (9)
O(2^{i})—Cu—O(4)	96·4 (8)	O(2^{i})—Cu—O(2^{ii})	92·2 (9)
O(3^{i})—Cu—O(4)	103·5 (8)	O(3^{i})—Cu—O(3^{ii})	88·2 (10)
O(4)—Cu—O(2^{ii})	96·4 (8)	O(4)—Cu—O(3^{ii})	103·5 (8)

Symmetry code: (i) $-x+1, -y, -z+1$; (ii) $-x+1, y+\frac{1}{2}, -z+1$; (iii) $x, -y+\frac{1}{2}, z$; (iv) $-x+\frac{1}{2}, y, z+\frac{1}{2}$; (v) $x-\frac{1}{2}, -y, -z+1\frac{1}{2}$; (vi) $x+\frac{1}{2}, -y, -z+\frac{1}{2}$; (vii) $-x+1\frac{1}{2}, y, z+\frac{1}{2}$; (viii) $-x+2, -y, -z+1$.

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