Fig. 2. Projection along the c axis of $Cr(H_2O)_6$ octahedra and non-bonded water molecules in $Cr_2P_6O_{18}.21H_2O$. The ring anions have been removed. $Cr(1)(H_2O)_6$ and $Cr(2)(H_2O)_6$ octahedra are superimposed in projection.

The $Cr(H_2O)_6$ *octahedra*. The chromium coordination polyhedra are all built by water molecules and do not share any corner or edge. The $Cr(1)(H_2O)_6$ octahedron has a disordered coordination already discussed in *Experimental*. Cr(2) located on the special position 6(*b*) is surrounded by O(W2), O(W3)

and O(W4) water molecules building an almost regular octahedron of symmetry 222. Cr(3) is located on the ternary axis; O(W5) and O(W6) are built around it in a quasi-regular octahedron with threefold internal symmetry.

In addition, it must be noted that O(W7), O(W8) and O(W9) water molecules are not involved in the associated cation polyhedra. Two of these molecules have thermal factors significantly larger than those belonging to the chromium coordination.

Main interatomic distances and bond angles in this arrangement as well as the hydrogen-bond scheme are reported in Table 2. Fig. 1 reports in projection along the c axis the arrangement of P_6O_{18} ring anions and Cr atoms while Fig. 2 gives in projection along the same axis the arrangement of $Cr(H_2O)_6$ octahedra and non-bonded water molecules.

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Structure of $Er_2Ba_3Cu_2PtO_{10}$

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Abstract. $M_r = 1228.7$, monoclinic, $C2/m$, $a = 12.465$ (3), $b = 5.795$ (1), $c = 7.362$ (1) Å, $\beta = 105.54$ (2)°, $V = 509.9$ (2) Å^3, $Z = 2$, $D_x = 8.01$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0.71073$ Å, $\mu = 45.8$ mm^{-1}, $F(000) = 960$, room temperature, final $R = 0.043$ for 982 $[|F_o| > 3\sigma(F_o)]$ unique reflections. The crystal is one of the compounds of rare-earth–barium–copper–platinum complex-oxides series and isomorphous with other $R_2Ba_3Cu_2PtO_{10}$ ($R = $ Y, Ho) oxides. In this compound, two distorted square pyramids of Cu^{II} and one distorted octahedron of Pt^{IV} are connected with each other by face sharing of the

polyhedra. The relationship between crystal structure and equilibrium stability of $R_2Ba_3Cu_2PtO_{10}$ and $R_2Ba_2CuPtO_8$ is discussed.

Introduction. Recently, a new series of quadruple oxides composed of rare earth, barium, copper, platinum and oxygen (RBCPO; $R = $ rare-earth elements) was found during the single-crystal growth of $RBa_2Cu_3O_{7-\sigma}$ superconductors by the CuO self-flux method. In this series two types of compounds, $R_2Ba_2CuPtO_8$ ($R = $ Ho, Er, Y; Saito, Ukei, Shishido & Fukuda, 1990; Ukei, Shishido & Fukuda, 1988; Laligant, Ferey, Hervieu & Raveau, 1987; Swinnea & Steinfink, 1987) and $R_2Ba_3Cu_2PtO_{10}$ ($R = $ Ho, Y; Geiser, Porter, Wang, Allen & Williams, 1988), have

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

$$B_{eq} = (4/3)\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
Pt	0·5	0	0·5	0·45
Er	0·3102 (1)	0	0·1265 (2)	0·51
Ba(1)	0·1509 (2)	0	0·5344 (3)	0·83
Ba(2)	0	0	0	0·67
Cu	0·4082 (4)	0	0·7943 (6)	0·57
O(1)	0·477 (2)	0·222 (4)	0·278 (3)	1·09
O(2)	0·317 (2)	0·230 (4)	0·874 (3)	0·94
O(3)	0·335 (2)	0	0·455 (4)	0·92

been studied. These compounds also grew in the same batch in this work.

Although platinum is usually hard to oxidize because of its high chemical potential energy, it was readily oxidized in air and formed complex oxides in our experiment. The incorporation mechanism of platinum from crucibles into these compounds is important in crystal growth.

Correlations between crystal structure and physical properties are interesting in view of the related superconductive compounds. In this study, the crystal structure of a new $R_2Ba_3Cu_2PtO_{10}$ compound (R = Er) has been reported.

Experimental. Crystals of $Er_2Ba_3Cu_2PtO_{10}$ have been obtained simultaneously with $Er_2Ba_2CuPtO_8$ by the CuO self-flux method. The detailed process of crystal growth was reported by Shishido, Fukuda, Toyota, Ukei & Sasaki (1987). Crystal size 0·38 × 0·25 × 0·1 mm; Rigaku AFC-6A four-circle diffractometer, graphite-monochromated Mo $K\alpha$ radiation; lattice parameters from 22 reflections ($61 < 2\theta < 65°$); ω–2θ scan mode, scan speed $4°$ $\min^{-1}$ (ω), data collection up to $2\theta = 65°$; three standard reflections with no significant intensity variation; 1920 reflections measured (h: $-18\rightarrow18$, k: $0\rightarrow8$, l: $-11\rightarrow11$), of which 982 unique reflections with $|F_o| > 3\sigma(F_o)$ are considered to be observed. $R_{int} = 0·054$, absorption correction ($14·91 < A^* < 235·06$); correction for Lorentz and polarization effects.

From the possible space groups (Cm, $C2$ and $C2/m$), $C2/m$ is adopted from the statistical distribution of the observed intensities. $C2/m$ proved to be the correct choice from later stages in the structure determination.

Under a hypothesis that this compound is isomorphous with $R_2Ba_3Cu_2PtO_{10}$ (R = Y, Ho), the structure was solved using the atomic parameters of the Ho compound in the first stage of structure determination. Refinement by full-matrix least squares on F of positional and anisotropic thermal parameters for all atoms converged to a final $R = 0·043$, $wR = 0·048$ [$w = 1/\sigma^2(F)$] and $(\Delta/\sigma)_{max} = 0·04$ in the last cycle. The final difference Fourier map shows

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

Pt—O(1)	2·03 (2)	Pt—O(2^{vii})	2·03 (2)
Pt—O(3)	2·00 (3)		
Cu—O(1^{vii})	2·10 (2)	Cu—O(2)	1·94 (2)
Cu—O(3)	2·41 (3)		
Pt—Cu	2·698 (6)		
Er—O(1)	2·44 (2)	Er—O(2^x)	2·30 (2)
Er—O(2^{xiv})	2·23 (2)	Er—O(3)	2·34 (3)
Ba(1)—O(1')	2·94 (2)	Ba(1)—O(1^{xiv})	2·86 (2)
Ba(1)—O(2)	3·08 (2)	Ba(1)—O(2^{xiv})	3·49 (2)
Ba(1)—O(3)	2·51 (3)	Ba(1)—O(3^{ii})	2·903 (2)
Ba(2)—O(1')	2·67 (2)	Ba(2)—O(2^{vii})	2·72 (2)

O(1)—Pt—O(1^{iv})	101·5 (8)	O(1)—Pt—O(1^{viii})	78·5 (8)
O(1)—Pt—O(3)	87·0 (9)	O(1^{vii})—Pt—O(3)	93·0 (9)
O(1^{vii})—Cu—O(2)	98·8 (9)	O(1^{vii})—Cu—O(2)	173·2 (8)
O(1^{vii})—Cu—O(3)	75·6 (9)	O(2)—Cu—O(3)	102·5 (8)
O(2)—Cu—O(2^{vi})	86·5 (9)		
O(1)—Er—O(3)	70·9 (8)	O(2^{xiv})—Er—O(3)	84·1 (7)
O(1)—Er—O(1^{iv})	63·6 (7)	O(2^x)—Er—O(2^{xiv})	89·5 (8)
O(1)—Er—O(2^{xiv})	152·7 (7)	O(1^{iv})—Er—O(2^{xiv})	98·4 (7)
O(1)—Er—O(2^x)	81·5 (7)	O(1)—Er—O(2^{xi})	117·6 (8)
O(2^{xiv})—Er—O(2^x)	125·8 (7)	O(2^{xiv})—Er—O(2^{xi})	76·7 (8)
O(2^x)—Er—O(3)	143·6 (5)	O(2^x)—Er—O(2^{xi})	70·7 (7)

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

max. and min. heights of 6·9 and $-6·7\,e\,\text{Å}^{-3}$. The value of g for the isotropic secondary extinction (Zachariasen, 1967) is $6·6\ (2) \times 10^{-5}$.

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, Vol. IV, pp. 79, 86, 90, 93, 149–150).

Discussion. Final atomic coordinates and selected interatomic distances and angles are presented in Tables 1 and 2.* The structure of the title compound is essentially analogous to other $R_2Ba_3Cu_2PtO_{10}$ (R = Y, Ho; Geiser *et al.*, 1988). A unit of coordination of Cu and Pt ions is shown in Fig. 1. Two distorted square pyramids of Cu^{II} and a distorted octahedron of Pt^{IV} are connected with each other by face sharing of the polyhedra. The distance from Cu^{II} to Pt^{IV}, 2·698 (6) Å, is shorter than the distance of Pt—Pt, 2·78 Å, in f.c.c. platinum metal. These units exist separately in the crystal lattice as shown in Fig. 2,

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53901 (7 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
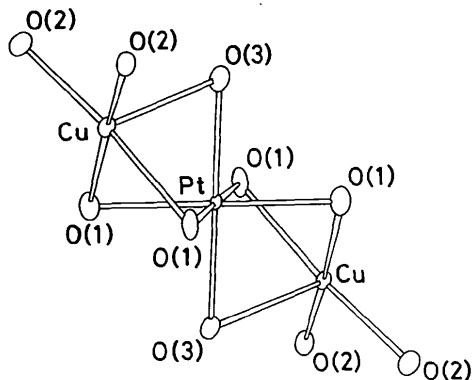
Fig. 1. The coordination geometry of the Pt and Cu ions, surrounded by O ions.

Fig. 2. Projection of the atomic arrangement of $Er_2Ba_3Cu_2PtO_{10}$ along the b axis.

while in $R_2Ba_2CuPtO_8$ the coordination polyhedra of Cu^{II} and Pt^{IV} are alternately connected sharing corners of the polyhedra to form one-dimensional chains (Saito *et al.*, 1990).

According to Pauling's third rule (Pauling, 1939), the presence of shared edges or particularly shared faces of coordination polyhedra around highly charged ions decreases the stability of the structure. Thus, the structure of $Er_2Ba_3Cu_2PtO_{10}$ with face-shared polyhedra seems to be less stable than the structure of $Er_2Ba_2CuPtO_8$ which is composed of corner-shared polyhedra. In the solid-state reaction at 1323 K, $Er_2Ba_3Cu_2PtO_{10}$ is formed first but gradually reacts with platinum and changes into Er_2Ba_2-$CuPtO_8$ after a long period (Saito, Shishido, Toyota, Ukei, Sasaki & Fukuda, 1991).
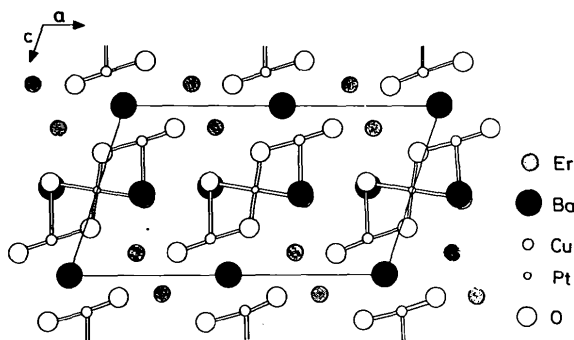
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Structure of Ammonium Trithio-*cyclo*-triphosphate

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Abstract. $(NH_4)_3[P_3O_6S_3]$, $M_r = 339.225$, orthorhombic, *Pnma*, $a = 12.450$ (8), $b = 12.755$ (8), $c = 8.154$ (6) Å, $V = 1294.9$ Å^3, $Z = 4$, $D_x = 1.739$ Mg m^{-3}, $\lambda(Ag\ K\bar{\alpha}) = 0.5608$ Å, $\mu = 0.480$ mm^{-1}, $F(000) = 696$, room temperature, final $R = 0.041$ for 1071 reflections. The $P_3O_6S_3$ ring anion has mirror symmetry. The S atoms are external atoms of the ring; two of them are located above the