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Structure of Erbium Pentaphosphate

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Abstract. ErP_5O_{14}, monoclinic, $C2/c$, $a = 12{\cdot}837$ (8), $b = 12{\cdot}723$ (7), $c = 12{\cdot}381$ (7) Å, $\beta = 91{\cdot}25$ (5)°, $M_r = 546{\cdot}1$, $V = 2021{\cdot}6$ Å^3, $Z = 8$, $D_x = 3{\cdot}59$, $D_m = 3{\cdot}55$ Mg m^{-3}, μ(Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å) $= 9{\cdot}49$ mm^{-1}. The final R factor with 2238 independent reflexions was 0·060. The structure is isomorphous with that of the monoclinic form of the holmium salt. Each crystallographically different Er^{3+} ion lies on a twofold axis and has eight O neighbours.

Introduction. It has been shown (Durif, 1971) that the crystal structure of a rare-earth pentaphosphate depends on the ionic radius of the rare-earth ion, but in all cases the individual rare-earth ions are well shielded, with no ions sharing the same oxygen, and the resulting minimum distance between rare-earth ions is not less than 5 Å. Mazurak, Ryba-Romanowski & Jeżowska-Trzebiatowska (1978) have reported the spectroscopic properties of ErP_5O_{14} single crystals. The present paper presents the crystal structure of ErP_5O_{14}, a possible highly concentrated laser material containing Er^{3+} ions.

The title compound was obtained as described by Mazurak *et al.* (1978). Weissenberg photographs showed that the crystals are monoclinic, space group $C2/c$ or Cc. A roughly cubic crystal, with edges of 0·15 mm, was selected for the data collection. A Syntex $P2_1$ diffractometer and Mo $K\alpha$ radiation with a graphite monochromator were used for lattice-parameter and intensity measurements. The intensities were measured by the 2θ–ω scan technique. After each group of 15 reflexions the intensity of a standard reflexion was measured; no significant change in intensity was observed. The data were corrected for Lorentz and polarization effects. Of the 2650 accessible reflexions in the range $10 \leq \theta \leq 30°$, 2238 with $I > 3\sigma(I)$ were used for the structure determination. All calculations were performed on a NOVA minicomputer with programs supplied by Syntex. Neutral-atom scattering factors

Table 1. *Final positional parameters of* ErP_5O_{14}

	x	y	z	B_{eq} (Å^2)
Er(1)	½	0·0317 (1)	¼	0·12
Er(2)	0	−0·0204 (1)	¼	0·13
P(1)	0·3224 (3)	0·2508 (3)	0·2405 (3)	0·38
P(2)	0·1496 (3)	0·1682 (3)	0·1030 (3)	0·13
P(3)	0·0253 (3)	0·3488 (3)	0·0324 (3)	0·18
P(4)	−0·1820 (3)	0·3628 (3)	0·1089 (3)	0·10
P(5)	−0·3535 (3)	0·4659 (3)	−0·0016 (3)	0·29
O(1)	0·3694 (9)	0·1500 (8)	0·2690 (8)	0·93
O(2)	0·5598 (8)	−0·0968 (8)	0·1330 (7)	0·55
O(3)	0·4747 (8)	0·1018 (8)	0·0745 (8)	0·84
O(4)	0·3469 (8)	−0·0490 (8)	0·1771 (8)	0·63
O(5)	−0·1163 (9)	−0·1567 (8)	0·2162 (8)	1·06
O(6)	0·0893 (8)	0·1296 (7)	0·1927 (7)	0·48
O(7)	−0·1143 (9)	0·0374 (8)	0·1149 (8)	0·86
O(8)	0·0763 (8)	−0·0654 (8)	0·0858 (8)	0·75
O(12)	0·2442 (8)	0·2360 (8)	0·1353 (8)	0·82
O(14)	0·2416 (8)	0·2729 (7)	0·3339 (8)	0·77
O(23)	0·0857 (8)	0·2392 (7)	0·0217 (7)	0·69
O(25)	0·1940 (7)	0·0818 (7)	0·0263 (7)	0·35
O(34)	−0·0910 (7)	0·3019 (7)	0·0550 (7)	0·30
O(45)	−0·2499 (9)	0·3963 (7)	0·0098 (7)	0·61

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used are those listed in *International Tables for X-ray Crystallography* (1974).

The heavy-atom method was employed for the phase determination. Approximate atomic positions were determined from three-dimensional Patterson and Fourier maps and later refined by a full-matrix least-squares program in space group $C2/c$. The final R and R_w were 0·060 and 0·072. The final atomic coordinates and their estimated standard deviations are listed in Table 1.* A final three-dimensional difference-Fourier synthesis was featureless.

The crystal structure is depicted in Fig. 1. Two-figure numbers at O atoms denote the numbers of the atoms bridged by the appropriate O atoms. The principal bond lengths and angles are presented in Table 2.

Table 2. *Interatomic distances* (Å) *and angles* (°) *with estimated standard deviations in parentheses*

Er(1)–O(1)	2·270 (10)	Er(1)–O(2)	2·326 (9)
Er(1)–O(3)	2·365 (9)	Er(1)–O(4)	2·377 (10)
Er(2)–O(5)	2·320 (10)	Er(2)–O(6)	2·344 (9)
Er(2)–O(7)	2·321 (10)	Er(2)–O(8)	2·347 (9)
O(1)–P(1)	1·457 (10)	O(2)–P(3)	1·484 (9)
O(3)–P(3)	1·465 (9)	O(4)–P(4)	1·448 (10)
O(5)–P(1)	1·451 (11)	O(6)–P(2)	1·453 (9)
O(7)–P(5)	1·454 (10)	O(8)–P(5)	1·477 (10)
O(12)–P(1)	1·638 (10)	O(12)–P(2)	1·535 (10)
O(14)–P(1)	1·596 (10)	O(14)–P(4)	1·555 (10)
O(23)–P(2)	1·602 (9)	O(23)–P(3)	1·570 (9)
O(25)–P(2)	1·568 (9)	O(25)–P(5)	1·630 (9)
O(34)–P(3)	1·638 (9)	O(34)–P(4)	1·564 (9)
O(45)–P(4)	1·549 (10)	O(45)–P(5)	1·601 (11)
O(1)–Er(1)–O(2)	141·8 (4)	O(1)–Er(1)–O(2)′	98·5 (4)
O(1)–Er(1)–O(3)	76·0 (4)	O(1)–Er(1)–O(3)′	75·0 (4)
O(1)–Er(1)–O(4)	73·7 (4)	O(1)–Er(1)–O(4)′	148·6 (4)
O(2)–Er(1)–O(3)	74·5 (4)	O(2)–Er(1)–O(3)′	142·8 (4)
O(2)–Er(1)–O(4)	75·0 (4)	O(2)–Er(1)–O(4)′	69·6 (4)
O(3)–Er(1)–O(4)	73·6 (4)	O(3)–Er(1)–O(4)′	127·4 (4)
O(1)–Er(1)–O(1)′	96·9 (4)	O(2)–Er(1)–O(2)′	90·7 (4)
O(3)–Er(1)–O(3)′	135·7 (4)	O(4)–Er(1)–O(4)′	128·9 (4)
O(5)–Er(2)–O(6)	150·6 (4)	O(5)–Er(2)–O(6)′	110·3 (4)
O(5)–Er(2)–O(7)	73·3 (4)	O(5)–Er(2)–O(7)′	139·6 (4)
O(5)–Er(2)–O(8)	86·6 (4)	O(5)–Er(2)–O(8)′	72·2 (4)
O(6)–Er(2)–O(7)	80·2 (4)	O(6)–Er(2)–O(7)′	69·8 (4)
O(6)–Er(2)–O(8)	73·8 (4)	O(6)–Er(2)–O(8)′	132·6 (4)
O(7)–Er(2)–O(8)	73·9 (4)	O(7)–Er(2)–O(8)′	115·6 (4)
O(5)–Er(2)–O(5)′	83·3 (4)	O(6)–Er(2)–O(6)′	71·0 (4)
O(7)–Er(2)–O(7)′	143·1 (4)	O(8)–Er(2)–O(8)′	151·7 (4)
Er(1)–O(1)–P(1)	149·5 (7)	Er(1)–O(2)–P(3)	138·9 (6)
Er(1)–O(3)–P(3)	171·6 (7)	Er(1)–O(4)–P(4)	139·0 (6)
Er(2)–O(5)–P(1)	156·7 (7)	Er(2)–O(6)–P(2)	141·2 (6)
Er(2)–O(7)–P(5)	148·0 (7)	Er(2)–O(8)–P(5)	147·3 (6)
O(1)–P(1)–O(5)	122·7 (6)	O(1)–P(1)–O(12)	109·6 (6)
O(1)–P(1)–O(14)	104·6 (6)	O(5)–P(1)–O(12)	104·7 (6)
O(5)–P(1)–O(14)	111·8 (6)	O(12)–P(1)–O(14)	101·5 (5)
O(6)–P(2)–O(12)	115·0 (6)	O(6)–P(2)–O(23)	113·9 (6)
O(6)–P(2)–O(25)	115·6 (5)	O(12)–P(2)–O(23)	104·1 (6)
O(12)–P(2)–O(25)	104·8 (5)	O(23)–P(2)–O(25)	102·0 (5)
O(2)–P(3)–O(3)	123·5 (6)	O(2)–P(3)–O(23)	109·8 (6)
O(2)–P(3)–O(34)	106·5 (5)	O(3)–P(3)–O(23)	106·8 (6)
O(3)–P(3)–O(34)	109·2 (6)	O(23)–P(3)–O(34)	98·1 (5)
O(4)–P(4)–O(14)	115·3 (6)	O(4)–P(4)–O(34)	116·7 (6)
O(4)–P(4)–O(45)	112·4 (6)	O(14)–P(4)–O(34)	102·1 (5)
O(14)–P(4)–O(45)	106·8 (6)	O(34)–P(4)–O(45)	102·2 (5)
O(7)–P(5)–O(8)	122·3 (6)	O(7)–P(5)–O(25)	109·1 (6)
O(7)–P(5)–O(45)	106·7 (6)	O(8)–P(5)–O(25)	108·7 (6)
O(8)–P(5)–O(45)	107·7 (6)	O(25)–P(5)–O(45)	100·1 (5)
P(1)–O(12)–P(2)	137·7 (7)	P(1)–O(14)–P(4)	142·6 (7)
P(2)–O(23)–P(3)	134·0 (7)	P(2)–O(25)–O(5)	128·6 (6)
P(3)–O(34)–P(4)	125·7 (6)	P(4)–O(45)–P(5)	132·4 (7)

Discussion. The crystals of ErP_5O_{14} are isomorphous with crystals of the monoclinic modification of HoP_5O_{14} (Bagieu, Tordjman, Durif & Bassi, 1973). However, the overall structure of ErP_5O_{14} is different from those of NdP_5O_{14} (Albrand, Attig, Fenner, Jeser & Mootz, 1974) and the orthorhombic modification of HoP_5O_{14} (Tranqui, Bagieu-Beucher & Durif, 1972).

In the ErP_5O_{14} crystals there are two crystallographically different Er atoms which lie on twofold axes. However, the coordination of both cations by O atoms is eightfold and may be described as a square antiprism. The nonequivalent positions of the Er atoms indicated by crystallographic studies do not seem to influence the emission and absorption spectra (Mazurak, Ryba-Romanowski & Jeżowska-Trzebiatowska, 1978). This is probably due to small differences in the first coordination sphere of the Er atoms.

The Er(1) and Er(2) atoms form zigzag chains along the crystallographic *c* axis, with Er(1)···Er(1) and Er(2)···Er(2) distances of 6·24 (1) and 6·21 (1) Å respectively. Both Er(1) and Er(2) atoms form further zigzag chains along the *a* axis with Er(1)···Er(2) distances of 6·45 (1) Å. In addition, the Er(1) and Er(2) atoms form linear chains along the *b* axis with

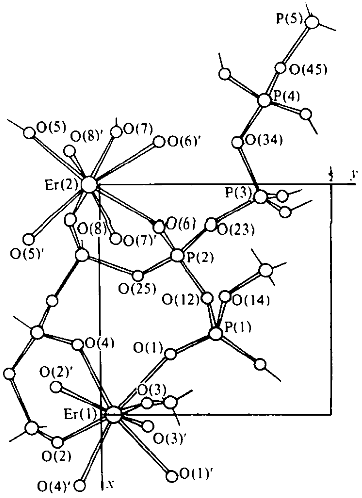

Fig. 1. View of part of the structure of ErP_5O_{14} down the *c* axis.

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35191 (43 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

alternating distances of 5·70 (1) and 7·02 (1) Å; that of 5·70 (1) Å is the shortest Er···Er distance in the structure.

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