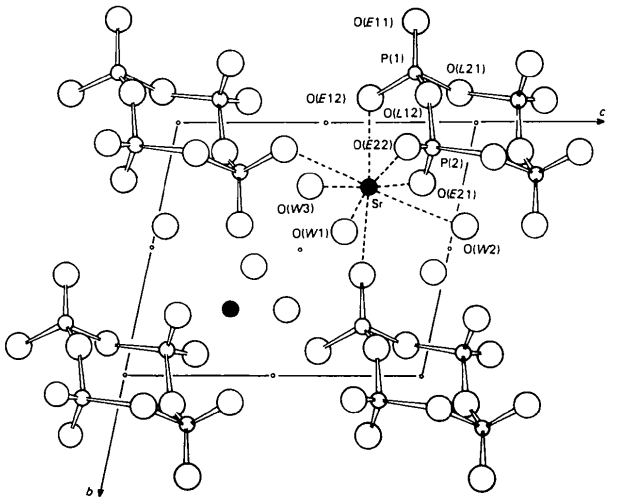

Fig. 1. Projection along the *a* axis of the atomic arrangement of $Sr_2P_4O_{12}.6H_2O$.

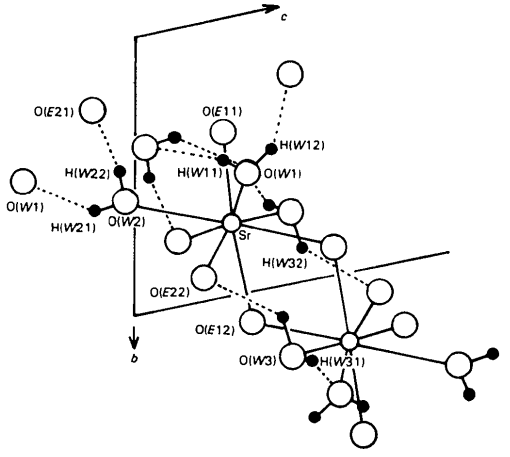

Fig. 2. Details of an $Sr_2O_8(H_2O)_6$ group in projection along the *a* axis. Hydrogen bonds are shown.

Table 2. *Main interatomic distances* (Å) *and bond angles* (°) *in the atomic arrangement of* $Sr_2P_4O_{12}.6H_2O$

The P_4O_{12} ring anion

$P(1)O_4$ tetrahedron

P(1)	O(*L*12)	O(*L*21)	O(*E*12)	O(*E*11)
O(*L*12)	1·616 (3)	2·545 (5)	2·534 (5)	2·458 (5)
O(*L*21)	103·7 (2)	1·621 (3)	2·484 (5)	2·550 (5)
O(*E*12)	109·3 (2)	105·8 (2)	1·490 (4)	2·574 (5)
O(*E*11)	105·4 (2)	110·9 (2)	120·5 (2)	1·474 (3)

$P(2)O_4$ tetrahedron

P(2)	O(*L*12)	O(*L*21)	O(*E*21)	O(*E*22)
O(*L*12)	1·620 (3)	2·466 (5)	2·547 (4)	2·489 (4)
O(*L*21)	99·7 (2)	1·606 (4)	2·531 (5)	2·505 (5)
O(*E*21)	109·9 (2)	109·6 (2)	1·491 (3)	2·588 (5)
O(*E*22)	106·5 (2)	108·3 (2)	120·8 (2)	1·485 (3)

P(1)–P(2)	2·951 (1)	P(1)–O(*L*12)–P(2)	131·6 (2)
P(1)–P(2)	2·916 (2)	P(2)–O(*L*21)–P(1)	129·3 (2)
P(2)–P(1)–P(2)	81·48 (4)	P(1)–P(2)–P(1)	98·52 (4)

SrO_8 polyhedron

Sr–O(*E*11)	2·541 (3)	Sr–O(*E*22)	2·596 (3)
Sr–O(*E*12)	2·644 (3)	Sr–O(*W*1)	2·627 (4)
Sr–O(*E*12)	2·593 (3)	Sr–O(*W*2)	2·683 (4)
Sr–O(*E*21)	2·632 (3)	Sr–O(*W*3)	2·623 (4)

Water molecules and hydrogen bonds

	O(*W*)–H	H···O	O(*W*)–O	O(*W*)–H···O	H–O(*W*)–H
O(*W*1)–H(*W*11)···O(*W*2)	0·80 (8)	2·09 (9)	2·858 (6)	161 (8)	109 (8)
O(*W*1)–H(*W*12)···O(*W*3)	0·80 (8)	2·14 (8)	2·832 (6)	144 (8)	
O(*W*2)–H(*W*21)···O(*W*1)	0·78 (9)	2·32 (9)	2·858 (6)	126 (8)	101 (8)
O(*W*2)–H(*W*22)···O(*E*21)	0·86 (10)	2·01 (9)	2·807 (5)	154 (8)	
O(*W*3)–H(*W*31)···O(*W*1)	0·92 (9)	2·02 (9)	2·832 (6)	150 (8)	93 (7)
O(*W*3)–H(*W*32)···O(*E*22)	1·00 (8)	1·92 (9)	2·895 (5)	166 (7)	

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Structure of Monobarium Tetracaesium Polyphosphate

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Abstract. $BaCs_4(PO_3)_6$, $M_r = 1142·79$, trigonal, $P3_1c$, $a = 11·549$ (5), $c = 9·114$ (5) Å, $V = 1052·8$ Å^3, $Z = 2$, $D_x = 3·604$ Mg m^{-3}, λ(Ag $K\alpha$) = 0·5608 Å, $\mu = 4·84$ mm^{-1}, $F(000) = 1020$, $T = 293$ K, final $R = 0·050$ for 894 independent reflexions. The $(PO_3)_\infty$ chains with a period of four tetrahedra are parallel to

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the c axis. The barium atoms and one of the caesium atoms, located on the internal threefold axes, have a ninefold oxygen coordination while caesium atoms in general positions have sevenfold coordination to oxygen.

Introduction. Barium caesium polyphosphate, $BaCs_4(PO_3)_6$, was characterized by Masse & Averbuch-Pouchot (1977) during the elaboration of the $Ba(PO_3)_2$–$CsPO_3$ phase equilibrium diagram. These authors reported the single-crystal preparation method and the main crystal data for this salt.

Table 1. *Final atomic coordinates and* B_{eq} *for* $BaCs_4(PO_3)_6$

$B_{eq} = \frac{4}{3}\sum_i\sum_j \mathbf{a}_i.\mathbf{a}_j\beta_{ij}$.

	x	y	z	B_{eq}(Å^2)
Ba	$\frac{1}{3}$	$\frac{2}{3}$	0·7592 (3)	1·64 (1)
Cs(1)	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$*	2·24 (1)
Cs(2)	0·2354 (1)	0·0069 (1)	0·5066 (2)	2·43 (1)
P(1)	0·5503 (4)	0·0057 (4)	0·0006 (6)	2·01 (5)
P(2)	0·3082 (4)	0·2847 (4)	0·2510 (7)	2·21 (6)
O(E11)	0·546 (1)	0·120 (1)	0·045 (2)	2·6 (2)
O(E12)	0·451 (1)	0·580 (1)	−0·024 (1)	2·0 (2)
O(L12)	0·382 (1)	0·426 (1)	0·337 (1)	3·0 (2)
O(E21)	0·162 (1)	0·209 (1)	0·271 (2)	3·4 (3)
O(E22)	0·392 (1)	0·221 (1)	0·267 (2)	2·2 (2)
O(L21)	0·346 (1)	0·319 (1)	0·586 (1)	3·2 (2)

* Fixed parameter.

Table 2. *Main interatomic distances* (Å) *and bond angles* (°) *in the atomic arrangement of* $BaCs_4(PO_3)_6$

$P(1)O_4$ tetrahedron

P(1)	O(E11)	O(E12)	O(L12)	O(L21)
O(E11)	1·405 (8)	2·568 (9)	2·406 (11)	2·588 (13)
O(E12)	120·7 (4)	1·548 (8)	2·505 (11)	2·549 (12)
O(L12)	104·1 (5)	103·5 (5)	1·641 (8)	2·518 (10)
O(L21)	117·4 (5)	107·0 (5)	101·1 (5)	1·621 (9)

$P(2)O_4$ tetrahedron

P(2)	O(E21)	O(E22)	O(L12)	O(L21)
O(E21)	1·474 (8)	2·589 (11)	2·598 (11)	2·403 (13)
O(E22)	121·8 (5)	1·489 (7)	2·513 (10)	2·596 (11)
O(L12)	114·4 (5)	108·0 (4)	1·616 (8)	2·436 (11)
O(L21)	100·8 (6)	112·0 (5)	96·8 (5)	1·642 (8)

P(1)–P(2)	2·914 (5)	P(1)–O(L12)–P(2)	127·2 (5)
P(2)–P(1)	2·917 (5)	P(2)–O(L21)–P(1)	126·6 (6)

$Cs(1)O_9$ polyhedron

Cs(1)–O(E11)	3·434 (9) (×3)
Cs(1)–O(E12)	3·228 (8) (×3)
Cs(1)–O(L12)	3·198 (7) (×3)

$Cs(2)O_7$ polyhedron

Cs(2)–O(E11)	3·212 (8)	Cs(2)–O(E22)	3·111 (8)
Cs(2)–O(E12)	3·176 (8)	Cs(2)–O(E22)	3·337 (8)
Cs(2)–O(E21)	2·988 (10)	Cs(2)–O(L21)	3·249 (9)
Cs(2)–O(E21)	3·106 (9)		

BaO_9 polyhedron

Ba–O(E11)	2·900 (9) (×3)
Ba–O(E12)	2·849 (8) (×3)
Ba–O(E22)	2·763 (8) (×3)

Experimental. Crystal used: hexagonal prism: $a = 0{\cdot}15$, $h = 0{\cdot}30$ mm; D_m not measured; Philips PW 1100 diffractometer; graphite monochromator; systematic absences: hhl with $l = 2n$; 20 reflexions ($12{\cdot}79 < \theta < 14{\cdot}66°$) for refining the unit cell; ω scan; scan speed: 0·02° s^{-1}; scan width: 1·20°; total background measuring time: 20 s; multiple scans for weak reflexions; intensity and orientation reflexions: 008 and 00$\bar{8}$ (no significant variation in intensity); θ range: 3–30°; 6198 reflexions measured ($\pm h$, $\pm k$, l); $h_{max} = 20$, $k_{max} = 20$, $l_{max} = 16$; 1250 non-zero independent reflexions (R_{int}: 0·031); Lorentz–polarization and absorption corrections (min., max. transmission coefficients: 0·36, 0·38); classical methods for structure determination: Patterson function and successive Fourier syntheses; anisotropic full-matrix least-squares refinement on F; unit weights; final refinements with 894 reflexions

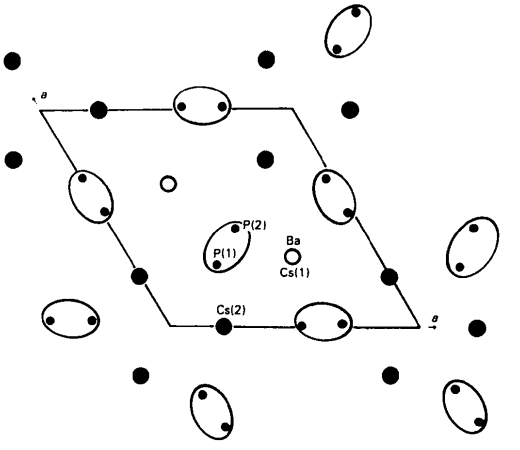

Fig. 1. Schematic representation of the respective locations of chains and associated cations in projection along the c axis. The chains are shown as ellipses.

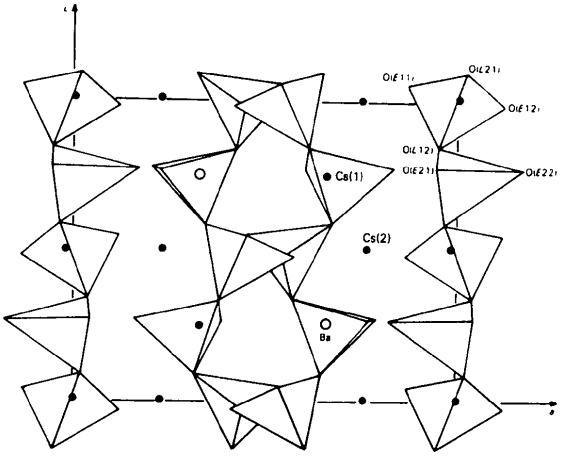

Fig. 2. Projection of the atomic arrangement of $BaCs_4(PO_3)_6$ along the a axis.

corresponding to $F_o > 5\sigma$; extinction refined: $g = 0{\cdot}74 \times 10^{-7}$ (Stout & Jensen, 1968). Final $R = 0{\cdot}050$ ($wR = 0{\cdot}053$); $S = 3{\cdot}431$; for the total set of 1250 reflexions $R = 0{\cdot}062$, $\Delta\rho_{max} = 1{\cdot}8$ e Å^{-3}, $(\Delta/\sigma)_{max} = 0{\cdot}06$ (extinction coefficient); scattering factors for neutral atoms and f', f'' from *International Tables for X-ray Crystallography* (1974); Enraf–Nonius (1977) *SDP* used for all calculations; PDP 11 Digital computer. Final refinements appeared to be very delicate because of very high correlation factors. Table 1 reports the final atomic coordinates.*

Discussion. The atomic arrangement can be described schematically as built up of infinite $(PO_3)_\infty$ chains parallel to the c axis interconnected by parallel rows of the associated cations. Fig. 1 is a schematic representation of the locations of the $(PO_3)_\infty$ chains and of the associated cation rows in projection along the c axis.

Fig. 2, a projection along the a axis, shows the main features of the chain anions.

Table 2 reports the main interatomic distances and bond angles in the phosphoric anion and in the associated cation polyhedra. The period of the $(PO_3)_\infty$ chain is four tetrahedra. Within a range of 3·5 Å Cs(1) and Ba atoms located on the internal threefold axes have nine oxygen neighbours while Cs(2) atoms on a general position have seven.

* Lists of observed and calculated structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42906 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of Mercury Potassium Trimetaphosphate

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Abstract. $HgKP_3O_9$, $M_r = 476{\cdot}6$, orthorhombic, $P2_12_12_1$, $a = 11{\cdot}164$ (6), $b = 12{\cdot}46$ (1), $c = 5{\cdot}622$ (2) Å, $V = 782{\cdot}0$ Å^3, $Z = 4$, $D_x = 4{\cdot}048$ Mg m^{-3}, $\lambda(Ag\ K\bar{\alpha}) = 0{\cdot}5608$ Å, $\mu = 11{\cdot}67$ mm^{-1}, $F(000) = 864$, $T = 293$ K, final $R = 0{\cdot}042$ for 1736 independent reflexions. The atomic arrangement is the same as that already described for barium sodium trimetaphosphate $BaNaP_3O_9$ but with an inversion of the cation valencies: Hg^{II} replacing Na and K replacing Ba. The KO_8 and HgO_6 polyhedra have average bond lengths K–O = 2·843 and Hg–O = 2·357 Å.

Introduction. During an investigation of $Hg(PO_3)_2$–M^IPO_3 systems, crystals corresponding to the formula $HgKP_3O_9$ were obtained. The unit-cell dimensions of this compound are close to those reported for barium sodium trimetaphosphate $BaNaP_3O_9$ (Martin & Mitschler, 1972). The common space group is $P2_12_12_1$. Given the respective sizes of the associated cations these analogies suggest an inversion of the cation valencies, mercury and potassium atoms replacing respectively sodium and barium atoms in the framework. Determination of the crystal structure of $HgKP_3O_9$ has been undertaken to verify this assumption.

Experimental. Single crystals of $HgKP_3O_9$ were obtained by a flux method. 2 g of mercuric oxide and 6 g of potassium dihydrogen monophosphate are introduced into 7 cm^3 of H_3PO_4 (85%). The resulting mixture is then heated at 623 K for four days. Large orthorhombic prisms of $HgKP_3O_9$, up to 5 mm long, are extracted by washing out the flux excess with hot water. A prism fragment cut to obtain an almost regular sphere ($R = 0{\cdot}13$ mm) was used for study. D_m not measured. Enraf–Nonius CAD-4 diffractometer. Graphite monochromator. Systematic absences: $h00$, $h = 2n$; $0k0$ $k = 2n$; $00l$, $l = 2n$. 22 reflexions ($10 < \theta < 13°$) for refining unit-cell dimensions. ω scan. 2

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