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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Acta Cryst. (1986). C**42**, 930–931

Structure of Mercury Potassium Trimetaphosphate

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(*Received* 6 *January* 1986; *accepted* 12 *March* 1986)

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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Table 1. *Final atomic coordinates for the atomic framework of* $HgKP_3O_9$

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

	x	y	z	B_{eq}(Å^2)
Hg	0·47903 (4)	0·13628 (3)	0·09635 (8)	1·051 (16)
K	0·1164 (2)	0·0795 (2)	0·0975 (6)	1·51 (5)
P(1)	0·4169 (2)	0·3719 (2)	0·3821 (6)	0·97 (5)
P(2)	0·3085 (2)	0·1862 (2)	0·5838 (6)	0·97 (5)
P(3)	0·1574 (2)	0·3572 (2)	0·3946 (6)	0·96 (5)
O(*L*13)	0·2831 (7)	0·4209 (6)	0·384 (2)	1·2 (2)
O(*L*12)	0·4083 (7)	0·2801 (6)	0·582 (2)	1·3 (2)
O(*E*11)	0·5014 (8)	0·4553 (7)	0·476 (2)	1·8 (2)
O(*E*12)	0·4449 (9)	0·3193 (8)	0·147 (2)	1·6 (2)
O(*L*23)	0·1882 (7)	0·2561 (7)	0·570 (2)	1·4 (2)
O(*E*21)	0·3176 (7)	0·1207 (7)	0·361 (1)	1·3 (2)
O(*E*22)	0·3149 (8)	0·1291 (8)	0·811 (2)	1·7 (2)
O(*E*31)	0·1277 (9)	0·3160 (8)	0·155 (2)	1·6 (2)
O(*E*32)	0·0687 (8)	0·4241 (8)	0·526 (2)	1·6 (2)

Table 2. *Main interatomic distances* (Å) *and bond angles* (°) *in* $HgKP_3O_9$

$P(1)O_4$ tetrahedron

P(1)	O(*L*13)	O(*L*12)	O(*E*11)	O(*E*12)
O(*L*13)	1·613 (5)	2·502 (7)	2·528 (7)	2·577 (7)
O(*L*12)	102·0 (3)	1·605 (6)	2·489 (7)	2·525 (8)
O(*E*11)	108·5 (3)	106·5 (3)	1·500 (5)	2·588 (8)
O(*E*12)	111·3 (3)	108·4 (3)	118·7 (3)	1·507 (6)

$P(2)O_4$ tetrahedron

P(2)	O(*L*12)	O(*L*23)	O(*E*21)	O(*E*22)
O(*L*12)	1·616 (5)	2·477 (6)	2·550 (7)	2·507 (8)
O(*L*23)	100·6 (3)	1·603 (5)	2·512 (7)	2·517 (8)
O(*E*21)	110·0 (3)	108·2 (3)	1·497 (5)	2·528 (7)
O(*E*22)	109·0 (3)	110·4 (3)	117·4 (3)	1·462 (6)

$P(3)O_4$ tetrahedron

P(3)	O(*L*13)	O(*L*23)	O(*E*31)	O(*E*32)
O(*L*13)	1·613 (5)	2·534 (7)	2·526 (7)	2·522 (7)
O(*L*23)	102·6 (3)	1·635 (5)	2·540 (8)	2·494 (7)
O(*E*31)	109·5 (3)	109·2 (3)	1·479 (6)	2·566 (8)
O(*E*32)	108·7 (3)	105·8 (3)	119·7 (3)	1·489 (6)

P(1)–P(2)	2·847 (2)	P(2)–P(1)–P(3)	60·98 (6)
P(1)–P(3)	2·903 (2)	P(1)–P(2)–P(3)	60·46 (6)
P(2)–P(3)	2·918 (2)	P(1)–P(3)–P(2)	58·56 (5)

P(1)–O(*L*13)–P(3)	128·3 (3)
P(1)–O(*L*12)–P(2)	124·2 (4)
P(2)–O(*L*23)–P(3)	128·6 (3)

HgO_6 polyhedron

Hg–O(*E*11)	2·302 (5)	Hg–O(*E*22)	2·439 (5)
Hg–O(*E*12)	2·329 (5)	Hg–O(*E*31)	2·259 (6)
Hg–O(*E*21)	2·346 (5)	Hg–O(*E*32)	2·467 (6)

KO_8 polyhedron

K–O(*E*11)	2·753 (6)	K–O(*E*22)	2·809 (6)
K–O*E*12)	2·674 (6)	K–O(*E*22)	2·964 (7)
K–O(*E*21)	2·740 (5)	K–O(*E*31)	2·967 (6)
K–O(*E*21)	2·920 (6)	K–O(*E*32)	2·916 (6)

standard reflexions, no intensity variation. 2380 reflexions measured ($3 < \theta < 30°$); h,k,l; $h_{max} = 19$, $k_{max} = 22$, $l_{max} = 8$. Scan width 1·30°, min. scan speed: 0·02° s^{-1}; max. background measuring time 35 s; Lorentz–polarization and absorption correction (min., max. transmission coefficients 0·16, 0·18). Structure by analogy with $BaNaP_3O_9$. Anisotropic full-matrix least-squares refinement (on F). Unit weights. Final refinement with 1736 reflexions corresponding to $F_o > 4\sigma_F$. Final $R = 0·042$ ($wR = 0·047$). $S = 3·219$. Max. $\Delta/\sigma = 0·001$ (extinction coefficient). Extinction coefficient refined to $g = 1·15 \times 10^{-7}$ (Stout & Jensen, 1968). $\Delta\rho_{max} = 2·09$ e Å^{-3}. Scattering factors for neutral atoms and f', f'' from *International Tables for X-ray Crystallography* (1974). Enraf–Nonius (1977) *SDP* used for all calculations. Computer used: Digital PDP 11.70. Table 1 reports the final atomic coordinates and B_{eq}*.

Discussion. As suggested in the *Introduction* the atomic framework for $HgKP_3O_9$ is strictly identical to that described for $BaNaP_3O_9$ by Martin & Mitschler (1972). The phosphoric anion is a trimeric one whose main geometrical features are reported in Table 2. The Hg and K atoms replace respectively Na and Ba atoms in the atomic arrangement of $BaNaP_3O_9$ without any significant distortions. The average Ba–O and Na–O distances observed for the BaO_8 and NaO_6 polyhedra in $BaNaP_3O_9$ are respectively 2·802 and 2·435 Å while in the title compound the average K–O and Hg–O distances in KO_8 and HgO_6 polyhedra are 2·843 and 2·357 Å.

* 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 42907 (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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