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SHORT STRUCTURAL PAPERS

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Structure of Mercury(II) Hydrogenphosphate

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Abstract. Synthetic $HgHPO_4$, $M_r = 296{\cdot}6$, triclinic, $P\bar{1}$, $a = 6{\cdot}288\,(2)$, $b = 7{\cdot}309\,(2)$, $c = 7{\cdot}276\,(2)$ Å, $\alpha = 79{\cdot}37\,(2)$, $\beta = 85{\cdot}27\,(2)$, $\gamma = 82{\cdot}85\,(2)°$, $V = 325{\cdot}5$ Å^3, $Z = 4$, $D_x = 6{\cdot}06$ Mg m^{-3}, μ(Mo $K\alpha$) = 47·65 mm^{-1}. The structure was solved by Patterson methods and refined to $R = 0{\cdot}041$ and $R_w = 0{\cdot}042$ for 1983 reflections having $I > 3\sigma(I)$ in the range $0{\cdot}40 < (\sin\theta)/\lambda < 0{\cdot}81$ Å^{-1}. The phosphate tetrahedra are linked in infinite chains by very strong hydrogen bonding. Each phosphate group participates in two hydrogen bonds. Two hydrogen bonds with O···O distances of 2·454 (12) and 2·518 (14) Å involve O atoms which are centrosymmetrically related, whereas the third hydrogen bond with an O···O distance of 2·495 (12) Å includes no centre of symmetry. The two independent Hg atoms have 2 + 4 and 2 + 5 coordination polyhedra. The pairs of short Hg—O bonds are approximately *trans* and average 2·07 Å.

Introduction. No definite synthesis or characterization of $HgHPO_4$ has been described in the literature so far. The compound precipitating under experimental conditions given by Klement & Haselbeck (1964) and identified as $HgHPO_4$ is claimed to be a mixture of $Hg_3(PO_4)_2$ and $Hg_2(H_2PO_4)_2$ (Nilsson, 1975). The analogous lead compounds, $PbHPO_4$ and its deuterated isomorph $PbDPO_4$, have recently been shown to be ferroelectric (Negran, Glass, Brickenkamp, Rosenstein, Osterheld & Susott, 1974). The ferroelectric transition mechanism in $PbHPO_4$ and related compounds appears to involve ordering of H atoms in strong O—H···O bonds. Since $HgHPO_4$ may show ferroelectric properties similar to $PbHPO_4$ and with a view to establishing its hydrogen-bonding system we have grown single crystals of $HgHPO_4$ and determined its crystal structure.

Colourless crystals were obtained from a solution of 10 g $Hg_3(PO_4)_2$ in 100 g 99% H_3PO_4 at 353 K. Chemical analysis and thermogravimetric measurements of the weight loss due to the liberation of water at about 413 K are in agreement with the composition $HgHPO_4$. The crystal selected for data collection was a parallelepiped with bounding planes (100), (001) and (010) and 0·18 × 0·16 × 0·14 mm in size. It was mounted such that the spindle axis was approximately parallel to **a***. A total of 4247 reflections in the range $0{\cdot}0492 < (\sin\theta)/\lambda < 0{\cdot}8087$ Å^{-1} were measured by the θ–2θ scan technique at 295 K on a Picker FACS-I diffractometer with graphite-monochromated Mo $K\alpha$ radiation ($\lambda = 0{\cdot}7107$ Å) at a take-off angle of 1·9°. A basic scan range of 1·8° (with allowance for α_1, α_2 dispersion) was used. A scan speed of 2·0° min^{-1} in 2θ with background measurements of 10 s at each end of the scan range was initially employed. For $(\sin\theta)/\lambda > 0{\cdot}618$ Å^{-1} the scan speed was 1·0° min^{-1} and background measurements were 20 s. Crystal orientation and unit-cell dimensions were determined by least-squares refinement of the setting angles of 12 automatically centred reflections in the range $0{\cdot}483 < (\sin\theta)/\lambda < 0{\cdot}590$ Å^{-1}. The intensities of three regularly monitored reflections showed no significant variation during data collection. After correction for absorption

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(μ = 47·65 mm^{-1}, transmission coefficients 0·0009–0·0676) the data were averaged assuming space group $P\bar{1}$ ($R_{\rm av}$ = 0·018) to give 2542 unique reflections of which 2300 were considered observed [$I > 3\sigma(I)$]. Lorentz and polarization corrections were applied in the usual way. The XRAY 70 program system (Stewart, Kundell & Baldwin, 1970) was used in conjunction with the CDC computer of the ETH Zürich. The structure was solved and developed by conventional Patterson, Fourier and least-squares refinement methods. The agreement factors were R = 0·050 and R_w = 0·062 for a model in which the 12 non-H atoms were assigned anisotropic thermal parameters. However, low-angle data showed rather poor agreement between $|F_o|$ and $|F_c|$; owing to the very high linear absorption coefficient, unavoidable errors in defining sufficiently precisely the crystal shape together with program limitations in choosing a finer grid size for Gaussian integration, the absorption correction for low-angle data remains suspect. Therefore data having $(\sin\theta)/\lambda$ < 0·40 Å^{-1} were omitted from final refinements which also had the effect of enhancing the relative contributions of the lighter atoms to $|F_c|$. These refinements, now with 1983 observed data, lowered the values for R and R_w to 0·041 and 0·042.[*] The weights used were $\sigma^{-1}(F_o)$ where the $\sigma(F_o)$ are derived from counting statistics. H atoms could not be unambiguously located in difference Fourier syntheses. Assuming space group $P\bar{1}$, the hydrogen-bonding network involves, in part, H atoms bridging centrosymmetrically related O atoms. This implies, either that these H atoms lie at centres of symmetry or that they are disordered. Therefore, the data were reprocessed without averaging and refinements in space group $P1$ initiated. Non-reasonable refinements and higher R indices resulted. Final atomic positions (space group $P\bar{1}$) with isotropic U values from the final cycle of isotropic refinement are given in Table 1 and selected bond distances and angles in Table 2.

Table 1. *Positional and thermal parameters* (Å^2 × 10^2) *with e.s.d.'s in parentheses*

	x	y	z	U[*]
Hg(1)	0·12495 (6)	0·16482 (6)	0·29934 (6)	1·34 (3)
Hg(2)	0·44481 (6)	0·20692 (7)	0·82592 (7)	1·66 (3)
P(1)	0·6124 (4)	0·2606 (4)	0·3129 (4)	1·00 (12)
P(2)	0·9433 (4)	0·2940 (4)	0·7903 (4)	0·92 (12)
O(11)	0·4521 (14)	0·1495 (14)	0·2340 (14)	1·25 (46)
O(12)	0·8086 (14)	0·1144 (13)	0·3617 (14)	1·17 (43)
O(13)	0·5034 (15)	0·3298 (13)	0·4887 (11)	1·28 (38)
O(14)	0·6690 (15)	0·4343 (13)	0·1747 (12)	1·53 (43)
O(21)	1·1261 (14)	0·2048 (13)	0·9172 (12)	0·86 (32)
O(22)	0·7772 (14)	0·1518 (12)	0·8215 (14)	1·20 (40)
O(23)	1·0320 (16)	0·3397 (13)	0·5874 (12)	1·37 (41)
O(24)	0·8384 (14)	0·4804 (11)	0·8492 (12)	1·31 (38)

[*] The U values and errors are from the final cycle of isotropic refinement.

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

(*a*) [Hg–O] polyhedra

Hg(1)–O(11)	2·067 (9)	Hg(2)–O(21)	2·060 (9)
Hg(1)–O(12)	2·066 (9)	Hg(2)–O(22)	2·077 (9)
Hg(1)–O(23)	2·639 (9)	Hg(2) O(13)	2·466 (8)
Hg(1)–O(24)	2·649 (8)	Hg(2)–O(14)	2·631 (10)
Hg(1)–O(21)	2·741 (9)	Hg(2)–O(11′)	2·711 (11)
Hg(1)–O(22)	2·610 (10)	Hg(2)–O(11)	2·924 (10)
Hg(1)–O(12′)	2·919 (9)		

O(11)–Hg(1)–O(12)	166·6 (4)	O(21)–Hg(2)–O(22)	160·6 (3)
O(23)–Hg(1)–O(21)	144·4 (3)	O(13)–Hg(2)–O(11)	163·0 (3)
O(23)–Hg(1)–O(22)	148·1 (3)	O(14)–Hg(2)–O(11′)	170·5 (3)
O(21)–Hg(1)–O(12′)	142·5 (3)	O(21)–Hg(2)–O(13)	114·0 (3)
O(12′)–Hg(1)–O(24)	143·2 (3)	O(21)–Hg(2)–O(11)	76·1 (3)
O(22)–Hg(1)–O(24)	134·0 (3)	O(21)–Hg(2)–O(14)	79·0 (3)
O(11)–Hg(1)–O(23)	109·1 (4)	O(21)–Hg(2)–O(11′)	101·5 (3)
O(11)–Hg(1)–O(21)	80·5 (3)	O(22)–Hg(2)–O(13)	84·9 (3)
O(11)–Hg(1)–O(22)	75·1 (4)	O(22)–Hg(2)–O(11)	86·7 (3)
O(11)–Hg(1)–O(12′)	90·8 (3)	O(22)–Hg(2)–O(14)	109·9 (3)
O(11)–Hg(1)–O(24)	79·9 (3)	O(22)–Hg(2)–O(11′)	72·6 (3)
O(12)–Hg(1)–O(23)	79·9 (4)	O(13)–Hg(2)–O(14)	80·3 (3)
O(12)–Hg(1)–O(21)	98·0 (3)	O(13)–Hg(2)–O(11′)	91·0 (3)
O(12)–Hg(1)–O(22)	92·0 (3)	O(11)–Hg(2)–O(14)	88·8 (3)
O(12)–Hg(1)–O(12′)	82·4 (3)	O(11)–Hg(2) O(11′)	100·6 (3)
O(12)–Hg(1)–O(24)	112·3 (3)		
O(23)–Hg(1)–O(12)	72·8 (3)		
O(23)–Hg(1)–O(24)	76·8 (3)		
O(21)–Hg(1)–O(22)	67·0 (3)		
O(21)–Hg(1)–O(24)	71·3 (3)		
O(22)–Hg(1)–O(12′)	75·5 (3)		

(*b*) [PO_4] tetrahedra

P(1)–O(11)	1·573 (11)	P(2)–O(21)	1·538 (9)
P(1)–O(12)	1·548 (9)	P(2)–O(22)	1·539 (10)
P(1)–O(13)	1·539 (9)	P(2)–O(23)	1·527 (9)
P(1)–O(14)	1·529 (9)	P(2)–O(24)	1·556 (9)

O(11)–P(1)–O(12)	104·2 (5)	O(21)–P(2)–O(22)	105·7 (5)
O(11)–P(1)–O(13)	108·5 (5)	O(21)–P(2)–O(23)	109·9 (5)
O(11)–P(1)–O(14)	112·8 (5)	O(21)–P(2)–O(24)	110·3 (5)
O(12)–P(1)–O(13)	111·5 (5)	O(22)–P(2)–O(23)	113·7 (6)
O(12)–P(1)–O(14)	113·2 (5)	O(22) P(2) O(24)	109·4 (5)
O(13)–P(1)–O(14)	106·7 (5)	O(23)–P(2)–O(24)	107·8 (5)

(*c*) Hydrogen bonding

O(13)···O(13′)	2·518 (14)	O(23)···O(23′)	2·454 (12)
O(14)···O(24)	2·495 (12)		

P(1)–O(13)···O(13′)	118·9 (5)	P(2)–O(23)···O(23′)	119·7 (5)
P(1)–O(14)···O(24)	133·0 (6)	P(2)–O(24)···O(14)	112·8 (4)

Discussion. The two crystallographically independent phosphate groups are linked in infinite chains by strong hydrogen bonding as indicated in Table 2 and illustrated in Fig. 1. Fig. 2 shows the packing of these chains within the unit cell of $HgHPO_4$. Since the exact positions of the H atoms could not be determined by this X-ray work, the nature of the hydrogen bond has to be discussed in terms of the O···O distances observed. The lower limit on the length of an O···O

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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 36190 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

hydrogen bond hitherto known is about 2·38 Å (Olovsson & Jönsson, 1976). 'Very short' OHO bonds may be defined as hydrogen bonds in which the O···O distance is less than 2·50 Å (Speakman, 1972). Therefore at least one of the three hydrogen bonds found in $HgHPO_4$ (O···O = 2·45, 2·50 and 2·52 Å) should be considered as a very strong hydrogen bond. With a crystallographically imposed centre of symmetry on the hydrogen bonds O(13)···O(13′) and O(23)···O(23′), three possibilities for the nature of these bonds exist (Olovsson & Jönsson, 1976). First, the bond is truly symmetrical with the proton vibrating about a single position of minimum energy at the centre of symmetry. The other two possibilities involve a static-statistical or a dynamical disorder of the H atoms between alternative positions close to the centre of symmetry.

In hydrogen-bonded ferroelectrics such as KH_2PO_4, positional ordering of disordered H atoms is known to occur at the transition temperature (Curie point). These order–disorder phase changes can be detected and characterized by differential scanning calorimetry (Dubler & Kopajtič, 1980). In $HgHPO_4$, however, the DSC curve gives no evidence of any phase transition down to 98 K whereby an ordering of disordered H atoms could be inferred.

Fig. 3 illustrates the stereochemistry around the Hg atoms. For Hg(2) the geometry is a distorted 2 + 4 elongated octahedron. The O(21)—Hg—O(22) angle involving the two short Hg—O bonds is 160·6 (3)°; angles among *cis*-related atoms are in the range 72·6 (3) to 114·0 (3)°. For Hg(1) the geometry is a distorted 2 + 5 polyhedron, the O(11)—Hg—O(12) angle is 166·6 (4)°; angles among *cis*-related atoms are in the range 67·0 (3) to 112·3 (3)°. Highly distorted and variable geometries have been observed previously in other simple Hg^{II} salts. In many such compounds two Hg—O bonds are approximately *trans* to one another and are much shorter than the remaining Hg—O bonds. The two short Hg—O bonds of Hg(1)—O(11) = 2·067 (9), Hg(1)—O(12) = 2·066 (9) Å and Hg(2)—O(21) = 2·060 (9), Hg(2)—O(22) = 2·077 (9) Å in $HgHPO_4$ are compared with some analogous distances in other 2 + 4 or 2 + 5 distorted Hg^{II} compounds in Table 3.

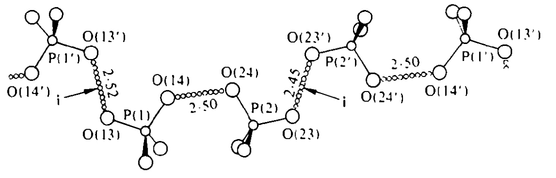

Fig. 1. Hydrogen-bonding scheme in $HgHPO_4$. PO_4 tetrahedra are linked in infinite chains by very strong hydrogen bonds. Centres of symmetry are denoted by i.

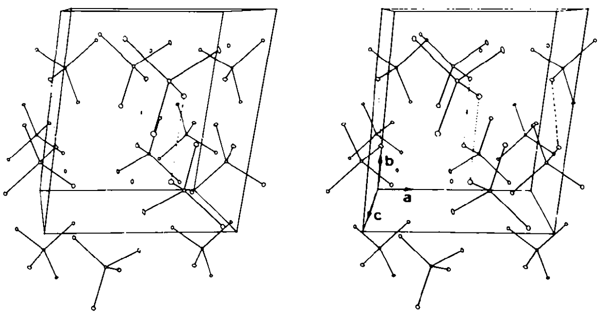

Fig. 2. The arrangement of phosphate and mercury ions in the unit cell. Hydrogen bonds are indicated by dashed lines.

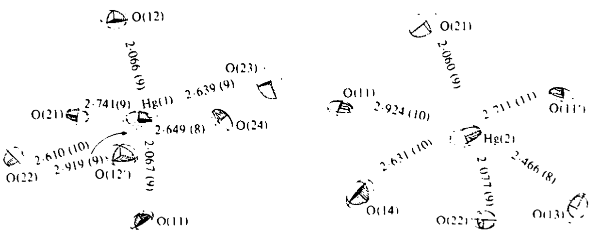

Fig. 3. The coordination sphere around the Hg atoms. Thermal ellipsoids are drawn at the 60% probability level. Distances are in Å.

Table 3. *Mean bond lengths* (Å) *and angles* (°) *of* 2 + 4 *or* 2 + 5 *distorted* Hg^{II}—O *polyhedra in non-chelated* Hg^{II} *compounds*

	Distortion	Hg—O_{short}	Hg—O_{long}	O—Hg—O_{short}	Reference
HgV_2O_6	2 + 4	2·01	2·43	180·0	*a*
$HgMoO_4$	2 + 4	2·026 (4)	2·719 (4)	180·0	*b*
HgO(hex.)	2 + 4	2·03 (2)	2·85 (2)	176 (3)	*c*
$Hg_2O(OH)(ClO_4)$	2 + 4*	2·05 (3)	2·78 (9)	171·8 (18)	*d*
HgO(orth.)	2 + 4	2·05 (3)	2·82 (3)	179·5 (11)	*e*
$HgHPO_4$	2 + 4	2·069 (9)	2·683 (10)	160·6 (3)	*f*
$HgLi_2(PO_3)_4$	2 + 4	2·133 (7)	2·517 (8)	165·1 (2)	*g*
$Hg_3(OH)_2(SO_4)_2.H_2O$	2 + 4	2·149	2·463	180·0	*h*
$HgSO_4.H_2O$	2 + 4	2·204 (2)	2·508 (1)	168·8 (1)	*i*
$Hg_2O(OH)(ClO_4)$	2 + 5*	2·02 (3)	2·74 (8)	172·8 (12)	*d*
$HgCrO_4.\frac{1}{2}H_2O$	2 + 5	2·060 (2)	2·698 (2)	180·0 (1)	*j*
$HgHPO_4$	2 + 5	2·066 (9)	2·712 (10)	166·6 (4)	*f*
$Hg(OH)NO_3$	2 + 5	2·086 (5)	2·718 (5)	171·6 (2)	*k*
$HgCrO_4$	2 + 5	2·109 (10)	2·596 (9)	163·3 (4)	*l*

References: (*a*) Angenault & Rimsky (1968); (*b*) Jeitschko & Sleight (1973); (*c*) Aurivillius & Carlsson (1958); (*d*) Johansson & Hansen (1972); (*e*) Aurivillius (1964); (*f*) this work; (*g*) Averbuch-Pouchot, Tordjman & Guitel (1976); (*h*) Aurivillius & Stålhandske (1976); (*i*) Stålhandske (1980); (*j*) Aurivillius & Stålhandske (1975); (*k*) Matković, Ribár, Prelesnik & Herak (1974); (*l*) Stålhandske (1978).

The e.s.d. (where available) for an individual parameter is given in parentheses. For the Hg—O_{long} separations the scatter of values about their mean is often large, especially in the case of 2 + 5 polyhedra.

* Other less easily categorized coordination polyhedra (approximately 2 + 6) are also observed in this structure.

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A Reinvestigation of the Structure of Sodium Hydrogenselenite

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Abstract. $NaHSeO_3$, monoclinic, $C2/c$, $a = 21{\cdot}9799$ (12), $b = 5{\cdot}7910$ (2), $c = 10{\cdot}2796$ (4) Å, $\beta = 105{\cdot}107$ (4)°, $V = 1263{\cdot}23$ Å^3, $Z = 16$, $d_x = 3{\cdot}17$ Mg m^{-3}, μ(Mo $K\alpha$) = 11·6 mm^{-1}, $R_w = 0{\cdot}0355$, $R = 0{\cdot}0259$. The refinement was based on F for 1924 reflexions. The structure comprises Na^+ ions and two independent hydrogen-bonded centrosymmetric $[HSeO_3]_2^{2-}$ dimers, linked to form a three-dimensional network by Na^+—O bonds. The structure can be considered as a superstructure having a pseudo-translation $\mathbf{e} = 1/2(\mathbf{a} + \mathbf{c})$.

Introduction. This investigation is part of a series of studies, in progress in Uppsala, of the crystal structures of alkali-metal trihydrogenselenites, $MH_3(SeO_3)_2$, and hydrogenselenites, $MHSeO_3$, respectively (M = alkali metal or NH_4^+) (Chomnilpan 1980*a*). In the hydrogenselenite series, the structures of $LiHSeO_3$ (Chomnilpan & Liminga, 1979) and $(NH_4)_2Se_2O_5$ (Chomnilpan, 1980*b*) have been reported. The hydrogenselenite does not exist for $M = NH_4^+$. Attempts to prepare the NH_4^+ hydrogenselenite result in the diselenite (Janickis, 1934). At Delft, interest in the study of $NaHSeO_3$ arose when it was found that intensities, derived from powder photographs, did not agree with calculated intensities based on the structure as reported by Chou, Hu & Yu (1963). A dimeric $[Se_2O_4(OH)_2]^{2-}$ ion with an unexpected configuration was reported to exist in this structure. Disagreement between the reported structure and results based on an NMR study have also been reported (Roslyakov & Vinogradova, 1979). There were therefore reasons to reinvestigate the structure of $NaHSeO_3$. According to the above-mentioned NMR study no phase transitions occur in the temperature range 133–333 K.

The cell dimensions were determined from a powder photograph recorded with a Guinier–Hägg XDC-700 focusing camera with Cr $K\alpha_1$ radiation ($\lambda = 2{\cdot}289753$ Å) and CoP_3 ($a = 7{\cdot}707780$ Å at 298 K) as an internal standard. A least-squares refinement based on the θ values of 45 reflexions provided the cell

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