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Structure of Strontium Tetrametaphosphate Hexahydrate

BY A. DURIF AND M. T. AVERBUCH-POUCHOT

Laboratoire de Cristallographie, Centre National de la Recherche Scientifique, Laboratoire associé à l'USMG, 166X, 38042 Grenoble CEDEX, France

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Abstract. $Sr_2P_4O_{12}.6H_2O$, $M_r = 599{\cdot}21$, triclinic, $P\bar{1}$, $a = 6{\cdot}644\ (3)$, $b = 7{\cdot}365\ (4)$, $c = 8{\cdot}618\ (4)$ Å, $\alpha = 101{\cdot}62\ (5)$, $\beta = 109{\cdot}98\ (5)$, $\gamma = 95{\cdot}65\ (5)°$, $V = 381{\cdot}7\ (4)$ Å^3, $Z = 2$, $D_x = 5{\cdot}213$ Mg m^{-3}, λ(Ag $K\alpha$) $= 0{\cdot}5608$ Å, $\mu = 8{\cdot}55$ mm^{-1}, $F(000) = 584$, $T = 293$ K, final $R = 0{\cdot}042$ for 1945 independent observed reflexions. Centrosymmetrical P_4O_{12} ring anions are located around the origin. They are linked in a three-dimensional way by $SrO_5(H_2O)_3$ polyhedra and hydrogen bridges. $SrO_5(H_2O)_3$ polyhedra link themselves pairwise so as to form $Sr_2O_8(H_2O)_6$ centrosymmetrical finite groups.

Introduction. Up to now the only example of a strontium cyclophosphate is given by the strontium trimetaphosphate heptahydrate: $Sr_3(P_3O_9)_2.7H_2O$ (Tordjman, Durif & Guitel, 1976). The present work is devoted to a structural investigation of strontium tetrametaphosphate hexahydrate: $Sr_2P_4O_{12}.6H_2O$.

Experimental. When diluted tetrametaphosphoric acid ($H_4P_4O_{12}$) is added to a water solution of strontium nitrate one observes after a few hours the formation of a polycrystalline crust at the bottom of the vessel. After a few days of slow evaporation at room temperature, large thick blades of $Sr_2P_4O_{12}.6H_2O$ develop at the surface of this crust. Crystals are stable for months at room temperature. Crystal size: $0{\cdot}30 \times 0{\cdot}24 \times 0{\cdot}18$ mm; density not measured; PW 1100 diffractometer, graphite monochromator; 15 reflexions ($10{\cdot}6 < \theta < 16{\cdot}5°$) for refining unit cell; $\omega/2\theta$ scan, scan speed: $0{\cdot}03°$ s^{-1}, scan width: $1{\cdot}40°$, total background measuring time: 16 s; intensity and orientation reflexions: 040 and $0\bar{4}0$ (no significant variations); θ range: 3–25°; 2692 reflexions measured, $h_{max} = \pm 11$, $k_{max} = \pm 13$, $l_{max} = 12$; Lorentz and polarization corrections, no absorption correction; classical methods for structure determination: Patterson function and successive Fourier syntheses; H atoms located from difference-Fourier synthesis; anisotropic full-matrix least-squares refinement on F for non-H atoms, isotropic for H atoms; unit weights; 2201 independent reflexions after rejection of those measured with an attenuator; final refinements with a set of 1945 reflexions corresponding to $F_o > 4\sigma_F$; final $R = 0{\cdot}042$ ($wR = 0{\cdot}051$), $S = 1{\cdot}430$; $\Delta\rho = 3{\cdot}3$ e Å^{-3}, $(\Delta/\sigma)_{max} < 0{\cdot}14$ [z of H(W21)]; scattering factors for neutral atoms and f' and f'' from *International Tables for X-ray Crystallography* (1974); Enraf–Nonius (1977) *SDP* used for all calculations; computer used: Digital PDP 11.70. Final atomic coordinates are reported in Table 1.*

Table 1. *Final atomic coordinates and isotropic thermal parameters for* $Sr_2P_4O_{12}.6H_2O$

B_{eq} are given for non-H atoms, B_{iso} for H atoms. $B_{eq} = \frac{4}{3}\sum_i\sum_j \mathbf{a}_i.\mathbf{a}_j\beta_{ij}$.

	x	y	z	B_{eq}/B_{iso}(Å^2)
Sr	0·59881 (8)	0·25201 (7)	0·69116 (6)	1·031 (2)
P(1)	0·2363 (2)	0·1960 (2)	0·2387 (2)	0·969 (8)
P(2)	0·8421 (2)	0·9056 (2)	0·1247 (2)	0·940 (8)
O(L12)	0·0216 (6)	0·8825 (5)	0·8242 (5)	1·27 (3)
O(L21)	0·7048 (6)	0·8855 (6)	0·9265 (5)	1·35 (3)
O(E11)	0·7417 (7)	0·5965 (5)	0·7254 (5)	1·74 (3)
O(E12)	0·6422 (6)	0·8946 (5)	0·6273 (5)	1·36 (3)
O(E21)	0·0062 (6)	0·2320 (5)	0·8588 (5)	1·34 (3)
O(E22)	0·3108 (6)	0·0872 (6)	0·7835 (5)	1·47 (3)
O(W1)	0·7340 (7)	0·5717 (6)	0·3568 (5)	1·92 (3)
O(W2)	0·7368 (8)	0·4064 (6)	0·0279 (6)	2·08 (4)
O(W3)	0·8182 (7)	0·2533 (6)	0·4895 (5)	1·96 (4)
H(W1)	0·74 (1)	0·50 (1)	0·27 (1)	3 (2)
H(W2)	0·75 (1)	0·52 (1)	0·43 (1)	3 (2)
H(W21)	0·78 (1)	0·39 (1)	0·12 (1)	3 (2)
H(W22)	0·83 (2)	0·50 (1)	0·04 (1)	4 (2)
H(W31)	0·03 (1)	0·73 (1)	0·47 (1)	3 (2)
H(W32)	0·79 (1)	0·15 (1)	0·39 (1)	3 (2)

Discussion. Fig. 1 is a projection along the a axis of the whole atomic arrangement.

The centrosymmetrical P_4O_{12} ring anion is located around the origin; geometrical details of this anion are given in Table 2.

The Sr atoms have an eightfold coordination made up of five O atoms and three water molecules. These $SrO_5(H_2O)_3$ polyhedra are linked pairwise, with a common edge [O(E12)–O(E12)], so as to form finite centrosymmetrical $Sr_2O_8(H_2O)_6$ groups. Fig. 2 gives, in projection along the a axis, the representation of such a unit. Main hydrogen-bond characteristics are reported in Table 2 and are illustrated in Fig. 2.

* Lists of structure factors and ansiotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42901 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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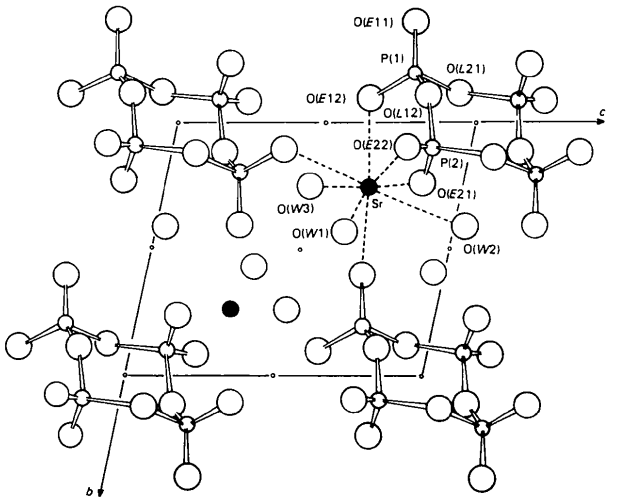

Fig. 1. Projection along the *a* axis of the atomic arrangement of $Sr_2P_4O_{12}.6H_2O$.

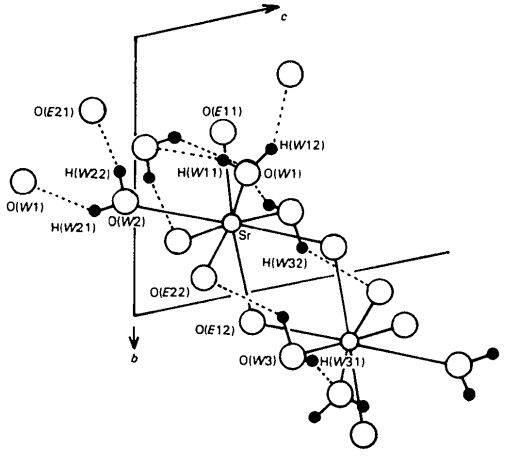

Fig. 2. Details of an $Sr_2O_8(H_2O)_6$ group in projection along the *a* axis. Hydrogen bonds are shown.

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

BY M. T. AVERBUCH-POUCHOT AND A. DURIF

Laboratoire de Cristallographie, Centre National de la Recherche Scientifique, Laboratoire associé à l'USMG, 166X, 38042 Grenoble CEDEX, France

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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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