Les anions cycliques P_4O_{12} situés autour des axes $\bar{4}$ se trouvent en $z = \frac{1}{2}$, exactement à mi-chemin entre les couches de polyèdres que nous venons de décrire assurant, de ce fait la cohésion tridimensionnelle de l'arrangement atomique.

La Fig. 1 donne une représentation de l'ensemble de cette structure en projection selon la direction **c**, tandis que le Tableau 2 rassemble les caractéristiques de l'anion P_4O_{12} et des polyèdres des cations associés.

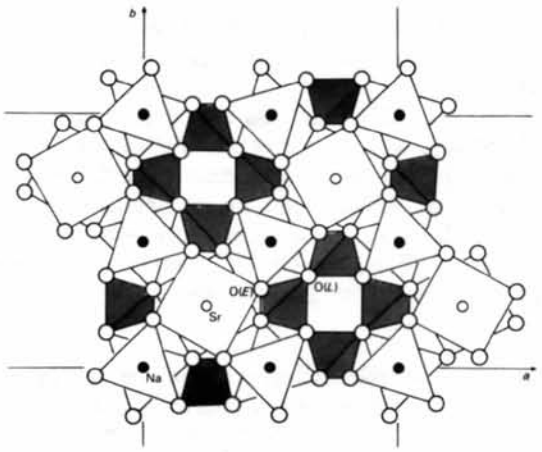

Fig. 1. Projection de l'arrangement atomique de $SrNa_2P_4O_{12}$ sur le plan *ab*. Les faces des tétraèdres de l'anion cyclique P_4O_{12} sont hachurées.

Tableau 2. *Principales distances interatomiques* (Å) *et angles de liaison* (°) *dans* $SrNa_2P_4O_{12}$

Le tétraèdre PO_4			
P–O(*E*)	1,480 (2)	O(*L*)–P–O(*L*)	102,98 (14)
P–O(*L*)	1,616 (2)	O(*L*)–P–O(*E*)	105,53 (10)
		O(*L*)–P–O(*E*)	110,27 (12)
		O(*E*)–P–O(*E*)	120,89 (13)
O(*L*)–O(*L*)	2,529 (6)		
O(*L*)–O(*E*)	2,541 (3)	P–P	2,956 (1)
O(*L*)–O(*E*)	2,466 (3)	P–O(*L*)–P	132,31 (4)
O(*E*)–O(*E*)	2,575 (3)		
L'octaèdre NaO_6			
Na–O(*L*)	2,685 (2) (× 2)		
Na–O(*E*)	2,334 (2) (× 4)		
L'antiprisme SrO_8			
Sr–O(*E*)	2,572 (2) (× 8)		

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Structure of Disodium Strontium Tetrametaphosphate Hexahydrate, $SrNa_2P_4O_{12}.6H_2O$

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Abstract. $M_r = 557{\cdot}6$, orthorhombic, *I*2*mm*, $a = 7{\cdot}332$ (5), $b = 7{\cdot}663$ (5), $c = 14{\cdot}408$ (8) Å, $V = 809{\cdot}5$ Å^3, $Z = 2$, $D_x = 2{\cdot}287$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}7107$ Å, $\mu = 4{\cdot}0$ mm^{-1}, room temperature, $F(000) = 552$, $R = 0{\cdot}033$ for 1033 independent reflexions. The structure comprises $P_4O_{12}^{4-}$ ring anions which show no unusual features, and SrO_8 antiprisms and NaO_6 octahedra which share a common face to form finite $SrNa_2O_8(H_2O)_6$ groups.

Introduction. Tetrametaphosphates corresponding to the general formula $M^{II}Na_2P_4O_{12}.xH_2O$ are not well known. Anhydrous disodium strontium tetrametaphosphate, $SrNa_2P_4O_{12}$, has been described previously (Averbuch-Pouchot & Durif, 1983). In the present study we describe the crystal structure of the hexahydrate of this salt. Crystals of $SrNa_2P_4O_{12}.6H_2O$ are readily prepared by mixing concentrated solutions of $Na_4P_4O_{12}.4H_2O$ and $Sr(NO_3)_2$ in an equimolar ratio. After some days, large prisms (up to 5 mm) of this salt appear in the solution.

Experimental. Cube-shaped crystal $0{\cdot}28 \times 0{\cdot}26 \times 0{\cdot}19$ mm, Nonius CAD-4 diffractometer, graphite-monochromated Mo $K\alpha$ radiation, ω-scan mode, scan width 1·6°, scan speed 0·04–0·01° s^{-1} according to intensity, total background measurement 19–62s, 15 reflexions used for measuring lattice parameters, no

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absorption correction, $2\theta_{max} = 70°$; $h_{max} = 11$, $k_{max} = 12$, $l_{max} = 23$; intensity reference reflexions (0,0,12 and 068) showed no appreciable variation; 1033 independent reflexions, 729 with $F_o > 3\sigma_F$ and $|F_o - F_c| > 37$ (F_o ranging from 0 to 711) [the second criterion eliminates 27 reflexions incorrectly measured (a failure of the so-called 'automatic attenuation system')], 277 unobserved. Structure solved using classical methods: study of a three-dimensional Patterson function, followed by successive Fourier syntheses; $\sum wAF^2$ minimized; H atoms not located; atomic coordinates, anisotropic thermal parameters and a scale factor refined; final $R = 0{\cdot}033$, $R_w = 0{\cdot}043$, $S = 0{\cdot}924$; unit weights; ratio of maximum least-squares shift to error 0·0 for final refinement cycle; maximum/minimum height in final difference Fourier map 0·2 e Å^{-3}; no correction for secondary extinction; atomic scattering factors and f', f'' values from *International Tables for X-ray Crystallography* (1974); Enraf–Nonius structure determination package.

Discussion. Table 1 gives the final atomic coordinates and equivalent isotropic thermal parameters.* Fig. 1 gives a projection of the atomic arrangement along **a**.

(*a*) *The* $P_4O_{12}^{4-}$ *ring anion.* These ring anions are located in planes $x = 0{\cdot}35$ and 0·85 and have *mm* symmetry. Table 2 reports their main geometrical features (interatomic distances and bond angles). They are not fundamentally different from what is commonly observed in other types of tetrametaphosphates.

(*b*) *The associated cations.* Na and Sr atoms are located in planes $x = 0{\cdot}0$, 0·12, 0·50 and 0·62; that is, almost half-way between planes of P_4O_{12} rings.

Sr atoms have an eightfold coordination of four O atoms [O(*E*2)] and four water molecules [O(*W*1) and O(*W*2)], forming a square antiprism. Na atoms are coordinated by a distorted octahedron of four O atoms [O(*E*1), O(*E*2)] and two water molecules [O(*W*2) and O(*W*3)]. It can be noted that only external O atoms [O(*E*)] contribute to the associated cation coordination. SrO_8 antiprisms and NaO_6 octahedra share a common face [2 × O(*E*2), O(*W*2)] to form finite $SrNa_2O_8(H_2O)_6$ groups. Table 2 reports the main interatomic distances in these groups.

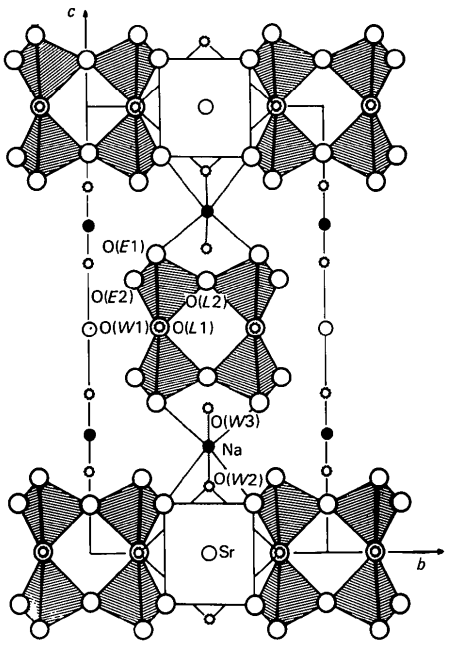

Fig. 1. Projection of the atomic arrangement of $SrNa_2P_4O_{12}.6H_2O$ along **a**. Water molecules sometimes superimposed on O atoms are indicated by snagged circles. P atoms belonging to the $P_4O_{12}^{4-}$ ring anions are not shown.

Table 2. *Selected interatomic distances* (Å) *and angles* (°)

$P_4O_{12}^{4-}$ anion

P	O(*E*1)	O(*E*2)	O(*L*1)	O(*L*2)
O(*E*1)	1·489 (5)	120·4 (3)	105·7 (3)	111·4 (3)
O(*E*2)	2·577 (7)	1·480 (4)	110·4 (3)	105·3 (3)
O(*L*1)	2·469 (4)	2·535 (6)	1·607 (3)	102·2 (3)
O(*L*2)	2·554 (7)	2·451 (4)	2·497 (7)	1·602 (3)

P–P	2·971 (3)	P–O(*L*1)–P	135·1 (4)
P–P	2·994 (2)	P–O(*L*2)–P	138·3 (4)

SrO_8 polyhedron		NaO_6 polyhedron	
4 × Sr–O(*E*2)	2·560 (4)	2 × Na–O(*E*1)	2·330 (5)
2 × Sr–O(*W*1)	2·574 (8)	2 × Na–O(*E*2)	2·384 (5)
2 × Sr–O(*W*2)	2·667 (7)	Na–O(*W*2)	2·797 (9)
		Na–O(*W*3)	2·356 (11)

Table 1. *Final atomic coordinates and equivalent isotropic thermal parameters, with e.s.d.'s in parentheses*

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

	x	*y*	*z*	B_{eq} (Å^2)
Sr	0	0	½	0·81 (2)
P	0·8494 (2)	0·1953 (2)	0·10311 (8)	0·87 (2)
Na	0·1175 (5)	0	0·2636 (2)	1·68 (9)
O(*E*1)	0·0072 (8)	0·2196 (5)	0·1669 (2)	1·74 (9)
O(*E*2)	0·1871 (6)	0·1907 (5)	0·3895 (3)	1·48 (9)
O(*L*1)	0·4326 (7)	0·2962 (7)	½	1·16 (12)
O(*L*2)	0·2722 (8)	½	0·6078 (4)	1·22 (12)
O(*W*1)	0·3321 (11)	0·2049 (10)	0	3·14 (21)
O(*W*2)	0·2789 (10)	½	0·1469 (5)	2·40 (18)
O(*W*3)	0·3924 (12)	0	0·1790 (8)	4·42 (31)

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38470 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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