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Contribution to the Crystal Chemistry of Tetrametaphosphates(II)[1]

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Chemical preparations and crystal structures of two hydrated forms of $CsNa_3P_4O_{12}$ are described. $CsNa_3P_4O_{12} \cdot 4H_2O$ with $a = 14.50(2)$, $b = 7.804(3)$, $c = 7.006(3)$ Å crystallizes in space group $Imm2$, $Z = 2$. The crystal structure has been determined using 745 independent reflexions with a final R value of 0.028 ($R = 0.040$ with the 934 collected reflexions), $CsNa_3P_4O_{12} \cdot 3H_2O$ with $a = 11.39(1)$, $b = 10.92(1)$, $c = 11.81(1)$ Å, $\beta = 95.24(5)°$ in $P2_1/c$, $Z = 4$. The crystal structure has been solved with 2975 independent reflexions with a final R-value of 0.018 ($R = 0.057$ with all the 6531 collected reflexions). In both structures there are four-membered rings built up with corner-sharing phosphate tetrahedron. For the tetrahydrate, the ring symmetry is mm whereas in the trihydrate, one observes two independent ring anions of symmetry $\bar{1}$. In both cases hydrogen atoms have been located and refined.

Introduction

Mixed alkali metal tetrametaphosphates are not very numerous. One can only mention the two crystalline forms of $Na_2K_2P_4O_{12} \cdot 2H_2O$ and one form of $Na_2(NH_4)_2P_4O_{12} \cdot 2H_2O$ and $Na_2Rb_2P_4O_{12} \cdot 2H_2O$ we recently described (*1*). In the present paper, we report a study of two new mixed alkali metal tetrametaphosphates: $CsNa_3P_4O_{12} \cdot 4H_2O$ and $CsNa_3P_4O_{12} \cdot 3H_2O$. They are the first evidence for the existence of tetrametaphosphates of mixed alkali metal with a 1/3 ratio.

Chemical Preparation and Crystal Data

An aqueous solution of sodium tetrametaphosphate, prepared by hydrolysis of P_4O_{10} at 0°C (*4*), is added with cesium carbonate until CO_2 evolution ceases. The resulting solution is then kept at room temperature and several successive precipitations occur. The first one is composed of monoclinic $Na_4P_4O_{12} \cdot 4H_2O$, the second one corresponds to the crystallization of large rectangular thick plates of $CsNa_3P_4O_{12} \cdot 4H_2O$, and the last one consists of large irregular prisms of the trihydrate.

The Weissenberg technique lead to initial values for the unit cell dimensions. These values were further refined against the angular data from powder diffraction. $CsNa_3P_4O_{12} \cdot 4H_2O$ is orthorhombic, $Imm2$ ($Z = 2$) with unit cell dimensions $a = 14.49(4)$, $b = 7.812(3)$, $c = 7.004(3)$ Å, $D_x = 2.472$, $V = 792.8$ Å^3.

The trihydrate $CsNa_3P_4O_{12} \cdot 3H_2O$ is

[1] Lists of F_o, F_c, and hkl and lists of anisotropic thermal parameters are available from the authors on request.

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TABLE I

INDEXED POWDER PATTERN FOR $CsNa_3P_4O_{12} \cdot 4H_2O$

$h\,k\,l$	d_{cal} (Å)	d_{obs} (Å)	I_{obs}	$h\,k\,l$	d_{cal} (Å)	d_{obs} (Å)	I_{obs}
2 0 0	7.24	7.24	47	5 0 1	2.678	2.675	34
1 1 0	6.88	6.88	47	4 2 0	2.656	2.657	22
1 0 1	6.31	6.30	20	0 2 2	2.607	2.607	3
0 1 1	5.21	5.21	6	4 0 2	2.518	2.517	12
2 1 1	4.23	4.23	9	2 2 2	2.453	2.453	5
3 1 0	4.11	4.11	15	0 3 1	2.441	2.439	9
3 0 1	3.976	3.976	37	2 3 1	2.313	2.312	5
4 0 0	3.622	3.621	2	1 0 3	2.305	2.306	6
0 0 2	3.502	3.504	15	3 3 0	2.292	2.292	3
1 2 1	3.320	3.319	100	0 1 3	2.237	2.236	9
2 0 2	3.153	3.152	60	5 2 1	2.208	2.208	13
1 1 2	3.121	3.120	50	6 1 1	2.191	2.190	9
4 1 1	2.975	2.978	68	5 1 2	2.147	2.146	9
3 2 1	2.786	2.787	2				
5 1 0	2.717	2.719	3				

TABLE II

INDEXED POWDER PATTERN FOR $CsNa_3P_4O_{12} \cdot 3H_2O$

$h\,k\,l$	d_{cal} (Å)	d_{obs} (Å)	I_{obs}	$h\,k\,l$	d_{cal} (Å)	d_{obs} (Å)	I_{obs}
1 1 0	7.86	7.86	21	3 1 2	2.943	2.942	33
$\bar{1}$ 1 1	6.74	6.74	9	0 0 4	2.942		
1 1 1	6.36	6.35	7	$\bar{3}$ 2 2	2.838	2.837	22
0 0 2	5.88	5.89	2	4 0 0	2.836		
2 0 0	5.67	5.67	2	$\bar{3}$ 1 3	2.763	2.763	3
0 2 0	5.46	5.45	3	0 4 0	2.728	2.729	11
0 2 1	4.95	4.95	15	$\bar{4}$ 1 1	2.727		
$\bar{1}$ 1 2	4.85	4.86	10	1 1 4	2.700	2.701	16
1 1 2	4.57	4.57	10	2 2 3	2.693	2.694	12
$\bar{2}$ 0 2	4.28	4.28	27	2 3 2	2.663	2.664	19
0 2 2	4.00	4.00	33	0 4 1	2.658	2.657	16
2 0 2	3.909	3.908	19	1 4 0	2.653	2.651	9
$\bar{1}$ 2 2	3.849	3.850	3	$\bar{4}$ 0 2	2.651		
1 2 2	3.702	3.702	4	$\bar{2}$ 1 4	2.635	2.632	9
2 1 2	3.680	2.676	5	$\bar{1}$ 3 3	2.633		
$\bar{1}$ 1 3	3.603	3.600	15	2 1 1	2.622	2.621	9
3 1 0	3.573	3.574	24	3 3 0	2.622		
$\bar{3}$ 1 1	3.504	3.505	6	$\bar{3}$ 3 1	2.594	2.592	54
1 3 0	3.464	3.465	25	0 2 4	2.590		
$\bar{2}$ 2 2	3.370	3.373	61	$\bar{1}$ 2 4	2.570	2.569	3
3 1 1	3.340	3.339	15	4 2 0	2.516	2.515	15
1 3 1	3.298	3.299	15	1 2 4	2.482	2.481	4
$\bar{3}$ 1 2	3.178	3.178	100	2 4 0	2.459	2.457	9
2 2 2	3.178			2 1 4	2.455		
$\bar{1}$ 3 2	3.022	3.022	6				

monoclinic $P2_1/c$, with $a = 11.392(8)$, $b = 10.913(5)$, $c = 11.818(7)$ Å, $\beta = 95.24(5)°$, $Z = 4$, $D_x = 2.596$, $V = 1463.1$ Å^3. Tables I and II report the indexed powder diagrams for these two salts.

Unit cell dimensions reported in the abstract are those refined from the angular data of the four-circle diffractometer. They have been used throughout the structure determinations and for the final interatomic distance calculations.

Structure Determinations

Table III reports the main parameters used for the two diffraction data collections. Lorentz-polarization correction has been made but no absorption correction was applied.

Both structures have been solved by using classical methods: location of the heavy atoms from a three-dimensional Patterson map followed by successive Fourier syn-

TABLE III

PARAMETERS USED FOR THE DIFFRACTION DATA COLLECTIONS

	$CsNa_3P_4O_{12} \cdot 4H_2O$	$CsNa_3P_4O_{12} \cdot 3H_2O$
Apparatus	Philips PW 1100	Enfraf-Nonius CAD 4
Monochromator	Graphite plate	Graphite plate
Wavelength (Å)	Mo$K\alpha$ (0.7107)	Ag$K\alpha$ (0.5608)
Scan mode	$\omega/2\theta$	$\omega/2\theta$
Scan speed (°/sec)	0.02	From 0.01 to 0.04
Total background measurement(s)	20	From 20 to 80
Scan width (°)	1.20	1.60
θ range (°)	3–35	3–35
Intensity reference reflexions	0 0 6, 0 0 $\bar{6}$	0.10.$\bar{2}$, 0.$\bar{1}$0.2
Number of collected reflexions	934	6531
H_{Max}, K_{Max}, L_{Max}	22, 12, 11	±23, 22, 24
Crystal size (mm)	0.24 × 0.24 × 0.16	0.32 × 0.32 × 0.32
μ (cm^{-1})	29	16
$F(100)$	568	1096
Cell constants	$a = 14.50(2)$ Å	$a = 11.39(1)$
	$b = 7.804(3)$	$b = 10.92(1)$
	$c = 7.006(3)$	$c = 11.81(1)$
		$\beta = 95.24(5)$
	(Single crystal, 16 reflexions, $15° < \theta < 18°$)	(Single crystal, 16 reflexions, $12° < \theta < 16°$)

theses. Hydrogen atoms have been located by difference-Fourier syntheses and refined isotropically. Full matrix refinements have been run using a unitary weighting scheme. Enraf-Nonius Structure Determination Package has been employed (*2*). Atomic scattering factors have been taken from International Tables for X-Ray Crystallography (Table 2.2B from Ref. (*3*)). Anomalous dispersion has been taken into account. All calculations have been run using cell dimensions reported in Table III.

$CsNa_3P_4O_{12} \cdot 4H_2O$

The final R value for the complete set of 934 independent reflexions is 0.040. This same factor decreases to 0.028 for a set of 745 reflexions corresponding to the following criteria:

(a) $F_o > 3\sigma_F$ (181 rejected reflexions)

(b) $|F_o - F_c| < 40$ in a F scale ranging from 0 to 930 (189 badly measured reflexions rejected).

Table IV reports the final atomic parameters.

TABLE IV

FINAL ATOMIC COORDINATES FOR $CsNa_3P_4O_{12} \cdot 4H_2O$

Atoms	$x(\sigma)$	$y(\sigma)$	$z(\sigma)$	$B_{eq}(\sigma)$
Cs	0.0000(0)	0.0000(0)	0.0000(0)	3.10(2)
P	0.10103(6)	0.1930(1)	0.4924(2)	0.96(2)
Na(1)	0.0000(0)	0.5000(0)	0.1864(6)	1.46(10)
Na(2)	0.2784(2)	0.0000(0)	0.7302(4)	1.39(6)
O(E1)	0.1673(2)	0.2161(5)	0.6537(5)	1.69(8)
O(E2)	0.3951(2)	0.1975(4)	0.8211(5)	1.61(8)
O(L1)	0.5000(0)	0.2996(6)	0.0899(6)	1.11(10)
O(L2)	0.6044(3)	0.5000(0)	0.9141(7)	1.28(10)
O(W1)	0.2110(4)	0.0000(0)	0.0389(8)	2.50(17)
O(W2)	0.1290(5)	0.5000(0)	0.9293(8)	2.90(18)
				B_{iso}
H(1)	0.230(6)	0.09(1)	0.09(1)	6.(2)
H(2)	0.354(6)	0.09(1)	0.37(1)	6.(2)

Note. Isotropic thermal factors are reported for hydrogen atoms while B_{eq} are given for nonhydrogen atoms. $B_{eq} = \frac{4}{3} \Sigma\Sigma_{ij} \vec{a}_i \cdot \vec{a}_j \cdot \beta_{ij}$.

TABLE V

FINAL ATOMIC COORDINATES FOR $CsNa_3P_4O_{12} \cdot 3H_2O$

Atoms	$x(\sigma)$	$y(\sigma)$	$z(\sigma)$	$B_{eq}(\sigma)$
Cs	0.24599(1)	0.22621(2)	0.77168(2)	2.716(2)
P(1)	0.19096(4)	0.98876(5)	0.03137(5)	1.12(1)
P(2)	0.01130(4)	0.18602(5)	−0.00139(5)	1.10(1)
P(3)	0.32137(4)	0.50783(5)	0.00100(5)	1.19(1)
P(4)	0.49428(5)	0.19685(5)	0.53014(5)	1.20(1)
Na(1)	0.50000(0)	0.00000(0)	0.00000(0)	1.73(3)
Na(2)	0.00000(0)	0.50000(0)	0.00000(0)	1.98(3)
Na(3)	0.88677(8)	0.37445(9)	0.21109(8)	1.81(2)
Na(4)	0.39201(8)	0.65797(9)	0.71500(8)	1.75(2)
O(E11)	0.2812(1)	0.0021(2)	0.9496(1)	1.88(4)
O(E12)	0.2241(1)	0.5598(2)	0.6463(1)	1.98(4)
O(E21)	−0.0018(1)	0.7030(1)	0.9305(1)	1.76(4)
O(E22)	0.0087(1)	0.1976(2)	0.8736(1)	1.92(4)
O(L12)	0.0850(1)	0.5887(1)	0.4666(1)	1.32(3)
O(L21)	0.8695(1)	0.6197(2)	0.4525(2)	1.91(4)
O(E31)	0.2050(1)	0.0014(2)	0.4358(2)	2.09(4)
O(E32)	0.6701(2)	0.4745(2)	0.8750(1)	2.22(4)
O(E41)	0.5401(1)	0.7351(2)	0.8567(1)	1.73(4)
O(E42)	0.5177(2)	0.2906(1)	0.4451(1)	2.02(4)
O(L34)	0.6066(2)	0.3890(2)	0.0596(2)	2.39(4)
O(L43)	0.3964(2)	0.3908(2)	0.9690(1)	2.12(4)
O(W1)	0.4900(2)	0.0256(2)	0.2046(2)	2.14(4)
O(W2)	0.9786(2)	0.0551(2)	0.2971(2)	2.79(5)
O(W3)	0.2528(2)	0.6928(2)	0.2805(2)	2.16(4)
				B_{iso}
H(11)	0.478(3)	0.401(3)	0.689(3)	3.1(7)
H(12)	0.457(3)	0.530(3)	0.243(3)	3.9(8)
H(21)	0.063(3)	0.563(4)	0.256(3)	4.3(8)
H(22)	0.010(3)	0.629(4)	0.187(3)	5.0(9)
H(31)	0.251(3)	0.640(3)	0.231(3)	3.4(7)
H(32)	0.261(3)	0.647(4)	0.334(3)	4.1(8)

Note. Isotropic thermal factors are reported for hydrogen atoms while B_{eq} are given for nonhydrogen atoms. $B_{eq} = \frac{4}{3} \Sigma\Sigma_{ij} \vec{a}_i \cdot \vec{a}_j \cdot \beta_{ij}$.

$CsNa_3P_4O_{12} \cdot 3H_2O$

At the final stage of refinement only 2975 reflexions have been kept. From the complete set of 6531 reflexions have been omitted:

(a) 3510 reflexions corresponding to $F_{obs} < 4\sigma_F$;

(b) 25 very strong reflexions measured with the so-called "automatic attenuator"; they correspond to $F_{obs} > 1475$ in a scale ranging from 0 to 2960;

(c) 21 badly measured reflexions corresponding approximately to $|F_{obs} - F_{cal}| > 50$ in the same scale.

For the remaining 2975 reflexions the final

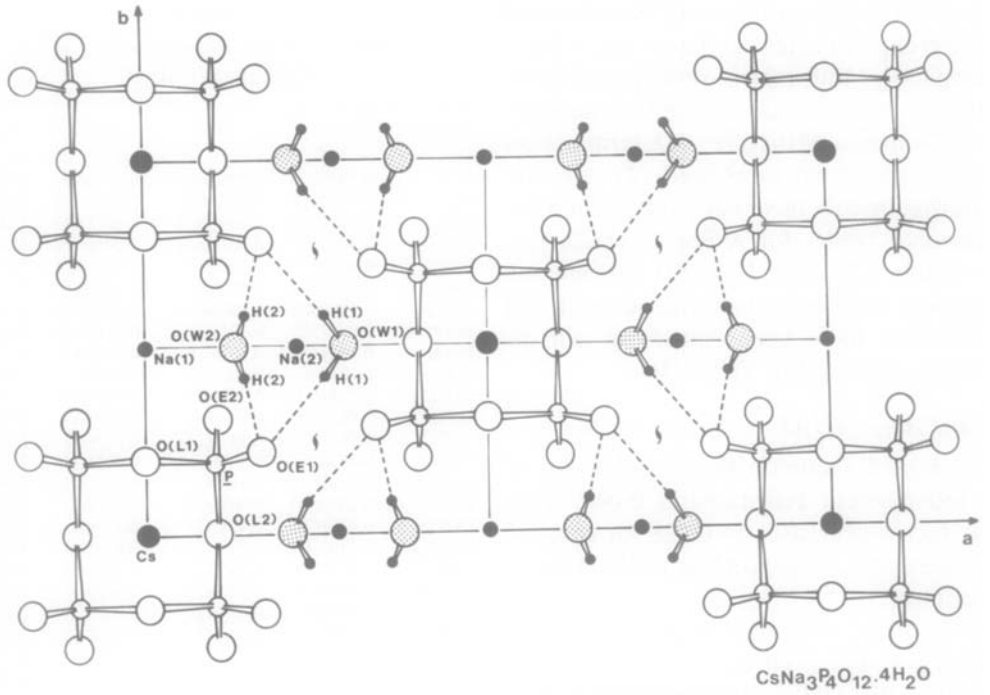

FIG. 1. Projection of the atomic arrangement of $CsNa_3P_4O_{12} \cdot 4H_2O$ along the $\vec{c}$ axis.

R value is 0.018, while this same factor is 0.057 for the complete set.

Table V reports the final atomic coordinates.

Structure Descriptions

$CsNa_3P_4O_{12} \cdot 4H_2O$

P_4O_{12} ring anions located around the twofold axis have *mm* symmetry, the four phosphorus atoms are so located in a plane perpendicular to the twofold $\vec{c}$ axis.

Groups of three distorted NaO_6 octahedra constituted by a central $Na(1)O_6$ octahedron sharing two faces with two $Na(2)O_6$ octahedra alternate with CsO_6 polyhedra in linear arrays parallel to the $\vec{a}$ axis. Both Na(1) and Na(2) are located on mirror planes. $Na(2)O_6$ octahedra and cesium polyhedra are connected by the O(W1) water molecule. Figure 1 reports a projection of this arrangement along the $\vec{c}$ axis.

The main geometrical features of the ring anion are reported in Table VI while Table VII gives the main interatomic distances in the associated cation polyhedra.

As shown in Fig. 1 the hydrogen bond bridges form discrete groups made of rings involving the two water molecules and two O(E1) oxygen atoms. It is to be noticed that the oxygen atoms O(E1) taking part in this scheme act twice as acceptors. Details of the hydrogen bond scheme are reported in Table VIII.

$CsNa_3P_4O_{12} \cdot 3H_2O$

The atomic arrangement of this second hydrate has no common feature with the first one. Here we observe two crystallographic independent P_4O_{12} ring anions, both centrosymmetrical. Figure 2, a projection of the atomic arrangement along the $\vec{c}$ axis, shows the disposition of these rings inside the unit cell, while Table VII reports their main geometrical features. The arrangement can be described as an alternating set

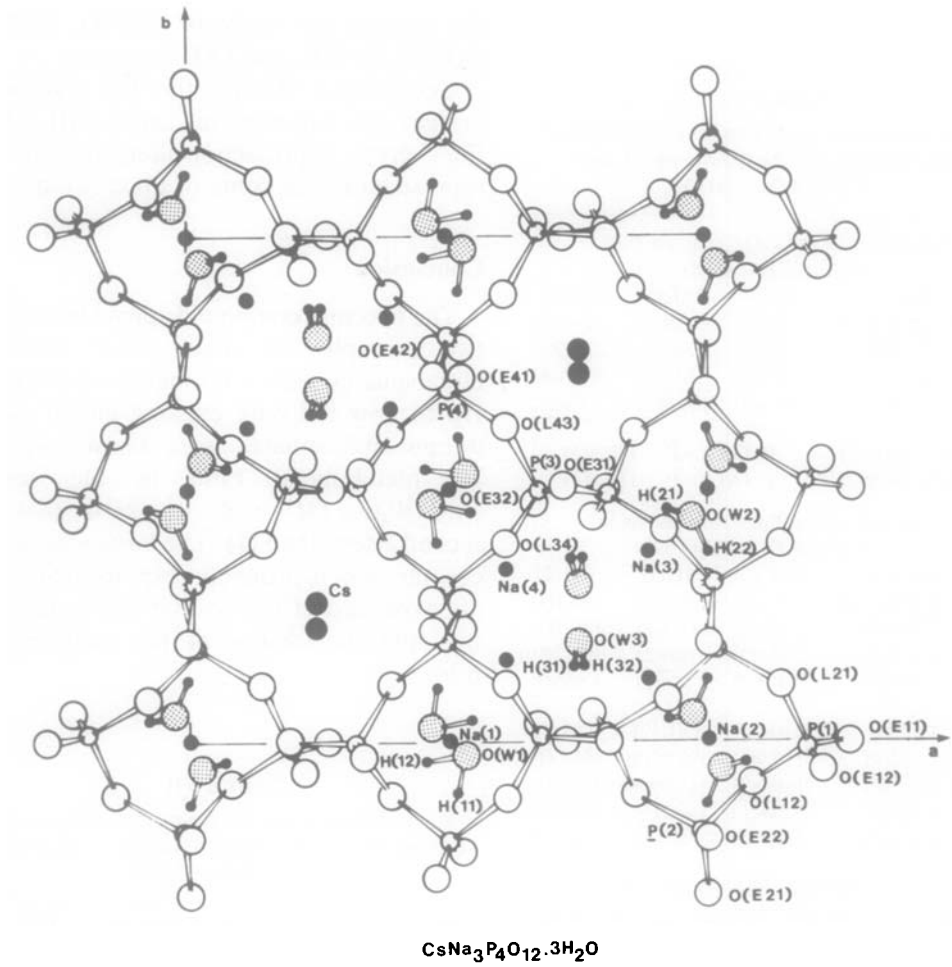

FIG. 2. Projection of the atomic arrangement of $CsNa_3P_4O_{12} \cdot 3H_2O$ along the $\vec{c}$ axis.

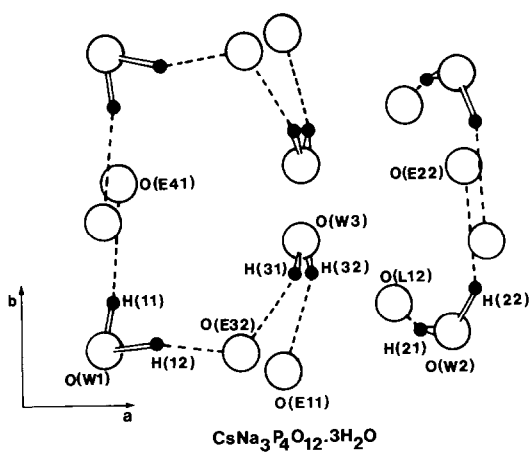

FIG. 3. Details of the hydrogen bond scheme in $CsNa_3P_4O_{12} \cdot 3H_2O$ projected along the $\vec{c}$ axis.

of P_4O_{12}–H_2O–Na–H_2O–P_4O_{12} rows, all parallel to the $\vec{c}$ axis. Between these rows one observes two types of channels, also parallel to the $\vec{c}$ axis, one of them containing the cesium atoms, the other one the Na(3) and Na(4) sodium atoms and the O(W3) water molecules. Both sodium and cesium atoms have a sixfold coordination. Cesium–oxygen and sodium–oxygen distances in these polyhedra are reported in Table VII.

As in the first hydrate, atoms involved in hydrogen bonds form discrete groups, but here of two different kinds: the first one made of O(W2), O(E22), and O(L12) atoms,

TABLE VI

MAIN GEOMETRICAL FEATURES OF THE P_4O_{12} RING ANIONS IN $CsNa_3P_4O_{12} \cdot 4H_2O$ AND $CsNa_3P_4O_{12} \cdot 3H_2O$

Geometry of the P_4O_{12} ring anion in $CsNa_3P_4O_{12} \cdot 4H_2O$

P	O(E1)	O(E2)	O(L1)	O(L2)
O(E1)	1.494(4) (Å)	2.589(6)	2.469(4)	2.548(6)
O(E2)	121.4(2)°	1.474(4)	2.548(6)	2.449(4)
O(L1)	105.0(3)	111.0(2)	1.617(2)	2.501(6)
O(L2)	110.6(3)	105.4(3)	101.9(3)	1.604(2)

P–P	3.012(2)	P–O(L1)–P	129.8(3)
P–P	2.929(2)	P–O(L2)–P	139.8(4)

Geometry of the P_4O_{12} ring anions in $CsNa_3P_4O_{12} \cdot 3H_2O$

P(1)	O(E11)	O(E12)	O(L12)	O(L21)
O(E11)	1.481(2) (Å)	120.1(1)	106.1(1)	108.7(1)
O(E12)	2.561(2)°	1.474(2)	111.5(1)	106.7(1)
O(L12)	2.471(2)	2.550(2)	1.609(2)	102.29(9)
O(L21)	2.510(2)	2.472(2)	2.504(2)	1.606(2)

P(2)	O(E21)	O(E22)	O(L12)	O(L21)
O(E21)	1.482(2)	119.9(1)	108.02(9)	105.6(1)
O(E22)	2.563(2)	1.480(2)	111.09(9)	109.8(1)
O(L12)	2.501(2)	2.546(2)	1.607(2)	100.62(9)
O(L21)	2.455(2)	2.520(2)	2.468(2)	1.599(2)

P(1)–P(2)	2.9720(8)	P(1)–O(L21)–P(2)	136.0(1)
P(2)–P(1)	2.9877(8)	P(2)–O(L12)–P(1)	136.5(1)
P(1)–P(2)–P(1)	93.83(2)	P(2)–P(1)–P(2)	86.17(2)

P(3)	O(E31)	O(E32)	O(L34)	O(L43)
O(E31)	1.474(2)	120.2(1)	106.7(1)	107.2(1)
O(E32)	2.554(2)	1.472(2)	111.3(1)	110.5(1)
O(L34)	2.468(2)	2.538(3)	1.601(2)	98.6(1)
O(L43)	2.478(2)	2.527(2)	2.428(3)	1.602(2)

P(4)	O(E41)	O(E42)	O(L34)	O(L43)
O(E41)	1.487(2)	119.7(1)	103.9(1)	110.2(1)
O(E42)	2.562(2)	1.475(2)	111.4(1)	105.7(1)
O(L34)	2.430(2)	2.540(3)	1.599(2)	105.1(1)
O(L43)	2.526(2)	2.445(2)	2.532(2)	1.591(2)

P(3)–P(4)	2.9780(8)	P(3)–O(L43)–P(4)	137.7(1)
P(4)–P(3)	2.9910(8)	P(4)–O(L34)–P(3)	138.4(1)
P(3)–P(4)–P(3)	86.12(2)	P(4)–P(3)–P(4)	93.88(2)

Note. For each tetrahedron diagonal underlined values correspond to P–O distances. Nondiagonal values correspond to O–P–O angles and O–O distances.

the second one made of O(E41), O(W1), O(E32), O(W3), and O(E11) atoms.

Geometrical details for the hydrogen bridges are reported in Table VIII while Fig. 3 gives, in projection along the $\vec{c}$ axis, a representation of some of these groups.

Conclusion

The two title compounds provide the first two examples of mixed alkali tetrametaphosphates with a 1/3 metal–metal ratio. Up to now the only existing mixed alkali tetrametaphosphates were known with a 1/1 metal–metal ratio in the series $Na_2M^I_2P_4O_{12}$ (M^I = K, Rb, NH_4) that we recently described (*1*). The large size of the cesium atom is probably responsible for the nonexistence of the cesium salt in this series and the change of the metal–metal ratio.

TABLE VII

MAIN INTERATOMIC DISTANCES IN ASSOCIATED CATION POLYHEDRA FOR $CsNa_3P_4O_{12} \cdot 4H_2O$ AND $CsNa_3P_4O_{12} \cdot 3H_2O$

Distances in cation polyhedra in $CsNa_3P_4O_{12} \cdot 4H_2O$ (Å)

CsO_6 polyhedron

Cs–O(L1)	3.272(5) (×2)		
Cs–O(L2)	3.272(6) (×2)		
Cs–O(W1)	3.071(8) (×2)		

NaO_6 polyhedra

Na(1)–O(E2)	2.362(4) (×4)	Na(2)–O(E1)	2.393(5) (×2)
Na(1)–O(W2)	2.596(9) (×2)	Na(2)–O(E2)	2.375(5) (×2)
		Na(2)–O(W1)	2.374(8)
		Na(2)–O(W2)	2.499(8)

Distances in cation polyhedra in $CsNa_3P_4O_{12} \cdot 3H_2O$ (Å)

CsO_6 polyhedron

Cs–O(E11)	3.226(2)	Cs–O(E32)	3.431(2)
Cs–O(E22)	3.074(2)	Cs–O(E41)	2.987(2)
Cs–O(L21)	3.307(2)	Cs–O(L43)	3.297(2)

NaO_6 octahedra

Na(1)–O(E11)	2.509(2) (×2)	Na(2)–O(E21)	2.363(2) (×2)
Na(1)–O(E42)	2.390(2) (×2)	Na(2)–O(E31)	2.520(2) (×2)
Na(1)–O(W1)	2.446(2) (×2)	Na(2)–O(W2)	2.462(2) (×2)
Na(3)–O(E12)	2.310(2)	Na(3)–O(E31)	2.386(2)
Na(3)–O(E21)	2.373(2)	Na(3)–O(W2)	2.505(2)
Na(3)–O(E22)	2.397(2)	Na(3)–O(W3)	2.550(2)
Na(4)–O(E12)	2.277(2)	Na(4)–O(L34)	2.710(2)
Na(4)–O(E41)	2.416(2)	Na(4)–O(W1)	2.303(2)
Na(4)–O(E42)	2.304(2)	Na(4)–O(W3)	2.448(2)

TABLE VIII

MAIN GEOMETRICAL FEATURES OF THE HYDROGEN BOND SCHEME IN $CsNa_3P_4O_{12} \cdot 4H_2O$ AND $CsNa_3P_4O_{12} \cdot 3H_2O$

	O(W)–H (Å)	H . . . O (Å)	O(W)–O (Å)	O(W)–H . . . O (°)	H–O(W)–H (°)
			$CsNa_3P_4O_{12} \cdot 4H_2O$		
O(W1)–H(1) . . . O(E1)	0.80(9)	2.19(9)	2.944(6)	155(10)	113(15)
O(W2)–H(2) . . . O(E1)	0.83(10)	2.19(11)	2.991(6)	162(11)	113(16)
			$CsNa_3P_4O_{12} \cdot 3H_2O$		
O(W1)–H(11) . . . O(E41)	0.83(4)	1.89(4)	2.725(3)	175(3)	101(3)
O(W1)–H(12) . . . O(E32)	0.83(4)	1.91(4)	2.740(3)	175(4)	
O(W2)–H(21) . . . O(L12)	0.76(4)	2.49(4)	3.154(3)	148(4)	99(4)
O(W2)–H(22) . . . O(E22)	0.84(5)	2.03(5)	2.858(3)	172(4)	
O(W3)–H(31) . . . O(E32)	0.82(4)	2.03(4)	2.789(3)	153(3)	97(4)
O(W3)–H(32) . . . O(E11)	0.81(4)	2.12(4)	2.916(3)	168(4)	

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