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The missing representatives of the hydrated sodium orthophosphate phases: $Na_3(PO_4)(H_2O)_7$ and $Na_3(PO_4)(H_2O)_6$

Matthias Weil[a]* and Berthold Stöger[b]

[a]Institute for Chemical Technologies and Analytics, Division of Applied Solid State Chemistry, Getreidemarkt 9/E164-05-1, 1060 Vienna, Austria, and [b]X-ray Centre, TU Wien, Getreidemarkt 9/E057-04, 1060 Vienna, Austria. *Correspondence e-mail: matthias.weil@tuwien.ac.at

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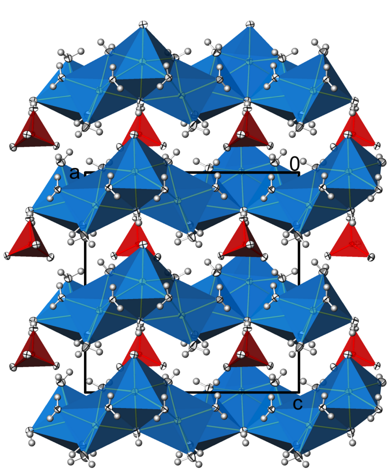
The crystal structures of the long-known compound $Na_3(PO_4)(H_2O)_6$, trisodium orthophosphate hexahydrate, and the compound $Na_3(PO_4)(H_2O)_7$, trisodium orthophosphate heptahydrate, the possible existence of which is discussed in the literature, were elucidated by single-crystal X-ray diffraction. In both crystal structures, all the water molecules are bound to the sodium cations, but the different water content leads to different arrangements in terms of polyhedral linkage. In the case of the heptahydrate (space group $Pca2_1$, $Z = 4$), this results in a layered structure made up from three sixfold coordinated Na^+ cations with phosphate units in between. In the case of the hexahydrate (space group $P\overline{1}$, $Z = 4$), a three-dimensional network is realised by one fivefold and five sixfold coordinated Na^+ cations, in which the phosphate units are embedded in the voids. In both crystal structures, the water molecules are involved in complex O—H$\cdots$O hydrogen-bonding networks and form moderately strong hydrogen bonds on average, almost exclusively with the phosphate O atoms. It is noteworthy that some O atoms accept up to five such bonds.



1. Chemical context

In continuation of our structural studies on $M_3(XO_4)(H_2O)_n$ compounds with tetrahedral anions (M = alkali metal; X = P, V), *viz*. $K_3(PO_4)(D_2O)_7$ (Weil & Stöger, 2020), $K_3(VO_4)(H_2O)_{0.56}$ and $K_3(VO_4)(H_2O)_4$ (Wolflehner & Weil, 2025), we became interested in the $Na_3(PO_4)(H_2O)_n$ system. Trisodium phosphate (TSP) and its hydrated phases are industrially relevant chemicals used on a large scale in the saponification of fats, as cleaning agents, or as water softening agents (Schrödter *et al.*, 2008). They are also used as food additives for their properties as complexing agents, acidity regulators, melting salts, emulsifiers or firming agents. Together with other sodium phosphates they are listed under the European approval number E339 for food additives (European Commission, 2025). Although TSP and its hydrate phases are well investigated due to these areas of application, there are still contradictions in the literature regarding the existence and composition of some hydrate phases (Menzel & von Sahr, 1937; Ingerson & Morey, 1943; Quimby, 1947; Bell, 1949; Wendrow & Kobe, 1952, 1954). For example, a compound with composition '$Na_3(PO_4)\cdot 12H_2O$' is still offered in the chemical trade, even though it has long been known that a phase with this composition does not exist because it contains additional NaOH and must be reformulated as $Na_3PO_4\cdot(NaOH)_{\simeq 0.25}\cdot 12H_2O$ (Tillmanns & Baur, 1970, 1971). Up to now, the existence of the hydrate phases $Na_3(PO_4)(H_2O)_8$, $Na_3(PO_4)(H_2O)_6$, and $Na_3(PO_4)(H_2O)_{0.5}$

Table 1
Selected bond lengths (Å) for $Na_3(PO_4)(H_2O)_7$.

Na1—O1	2.3010 (8)	Na2—O3*W*	2.4146 (7)
Na1—O1*W*	2.3146 (7)	Na2—O5*W*	2.4279 (7)
Na1—O2*W*	2.3440 (7)	Na2—O4*W*^{i}	2.6357 (7)
Na1—O3*W*	2.4413 (8)	Na3—O4*W*	2.3605 (7)
Na1—O4*W*^{i}	2.4626 (7)	Na3—O7*W*	2.3606 (7)
Na1—O5*W*^{ii}	2.5311 (7)	Na3—O2*W*^{iii}	2.3656 (8)
Na2—O1*W*	2.2991 (7)	Na3—O3*W*^{iii}	2.4421 (8)
Na2—O6*W*	2.3093 (8)	Na3—O5*W*^{iv}	2.4439 (7)
Na2—O7*W*	2.3558 (7)	Na3—O6*W*^{iv}	2.6575 (10)

Symmetry codes: (i) $x, y-1, z$; (ii) $x+\frac{1}{2}, -y+1, z$; (iii) $x-\frac{1}{2}, -y+2, z$; (iv) $x, y+1, z$.

has been unequivocally confirmed (Wendrow & Kobe, 1954), but only the crystal structures of the octahydrate (Larbot & Durand, 1983) and the hemihydrate (Averbuch-Pouchot & Durif, 1983) have been determined so far. In the older literature, the existence of $Na_3(PO_4)(H_2O)_7$ has been suggested by some authors (Menzel & von Sahr, 1937; Ingerson & Morey, 1943), but questioned by others (Quimby, 1947; Bell, 1949). In a more recent investigation of the thermal dehydration of '$Na_3(PO_4)\cdot12H_2O$', the heptahydrate phase of TSP was reported to appear as an intermediate dehydration product as revealed by temperature-dependent Raman studies (Ghule *et al.*, 2001).

In this article, we report on the crystal structures of the long-known compound $Na_3(PO_4)(H_2O)_6$ and of the suspected $Na_3(PO_4)(H_2O)_7$, thereby confirming the existence of the heptahydrate phase of TSP.

2. Structural commentary

2.1. $Na_3(PO_4)(H_2O)_7$

$Na_3(PO_4)(H_2O)_7$ crystallizes in the non-centrosymmetric orthorhombic space group *Pca*2$_1$, and the absolute structure of the crystal chosen for data collection has been reliably determined [Flack parameter 0.00 (3)]. The asymmetric unit comprises one formula unit. The crystal structure consists of three Na^+ cations sixfold surrounded by five water molecules and one phosphate O atom for Na1, and by six water molecules for both Na2 and Na3 (Fig. 1). By sharing edges and corners defined by water molecules, these polyhedra are linked into a layer structure extending parallel to (001), Fig. 2. Thereby, three water molecules (O*W*3, O*W*4, O*W*5) are bound to three Na^+ cations, and four (O*W*1, O*W*2, O*W*6, O*W*7) to two Na^+ cations each (Table 2). The isolated $[PO_4]^{3-}$ tetrahedra are sandwiched between layers (Table 1, Fig. 3), with only one of the phosphate oxygen atoms (O1) directly bound to a sodium cation.

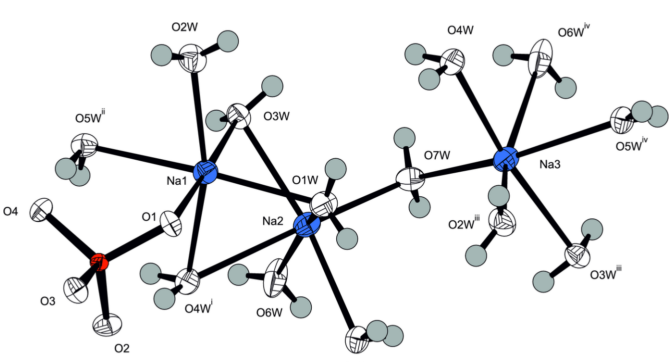


Figure 1
The asymmetric unit of $Na_3(PO_4)(H_2O)_7$ expanded to show the full coordination environments of the three Na^+ cations. Displacement ellipsoid are given at the 90% probability level except for H atoms, which are shown with an arbitrary radius. Symmetry codes refer to Table 1.

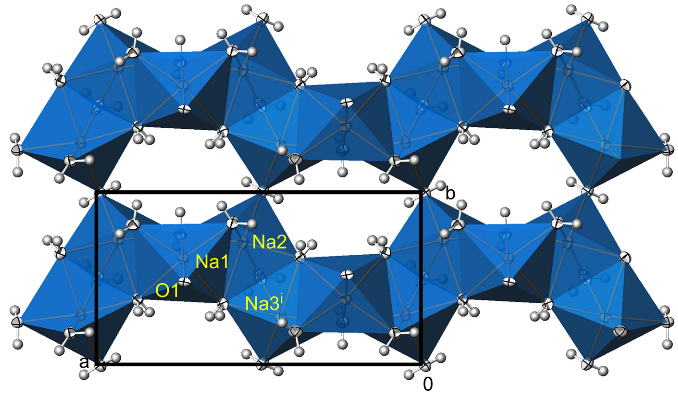


Figure 2
$Na_3(PO_4)(H_2O)_7$. Linkage of $[NaO(H_2O)_5]$ (Na1) and $[Na(H_2O)_6]$ (Na2, Na3) polyhedra into (001) layers in a view along [00$\overline{1}$]. Displacement ellipsoids are as in Fig. 1. [Symmetry code: (i) $x, 1-y, z$.]

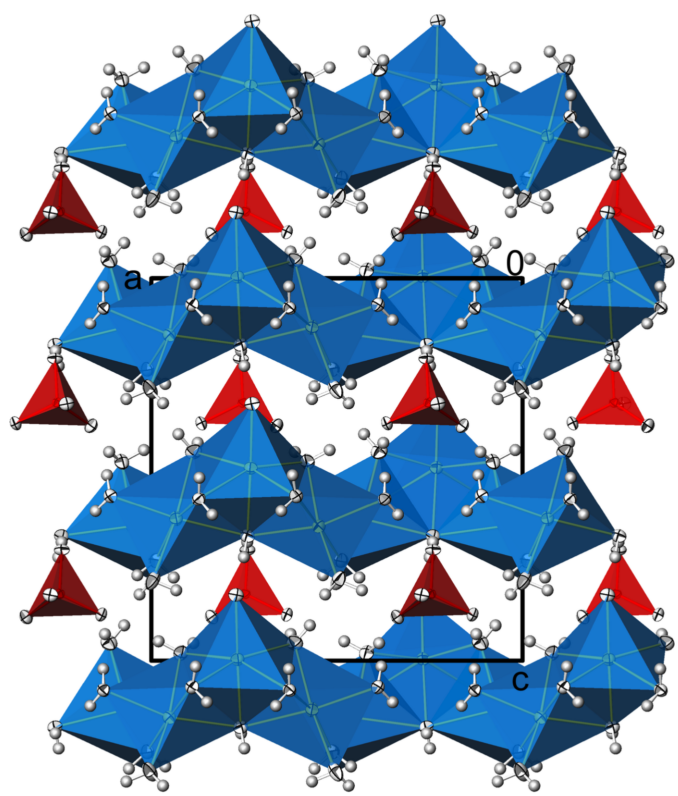


Figure 3
$Na_3(PO_4)(H_2O)_7$. View of the crystal structure along [0$\overline{1}$0], showing the $[PO_4]^{3-}$ tetrahedra in between the cationic layers. Displacement ellipsoids are as in Fig. 1.

Table 2
Coordination environments in $Na_3(PO_4)(H_2O)_7$ and $Na_3(PO_4)(H_2O)_6$, and results of BVS calculations (H atoms not taken into account).

Atom	Number of coordination partners	Polyhedron (idealized point group symmetry; deviation δ from it)	Range of M—O bond lengths (Å)	Average M—O bond length (Å)	Number of water molecules in the first coordination sphere (Na—O < 3.0 Å); *number of accepted hydrogen bonds*	BVS (v.u.)
$Na_3(PO_4)(H_2O)_7$						
Na1	6	Bailar twist (dynamic) (32; 6.105)	2.3009 (8)–2.5307 (8)	2.399	5	1.19
Na2	6	Bailar twist (dynamic) (32; 7.566)	2.2989 (8)–2.6359 (8)	2.407	6	1.16
Na3	6	Bailar twist (dynamic) (32; 7.357)	2.3604 (8)–2.6575 (10)	2.438	6	1.08
P1	4	tetrahedron ($\bar{4}3m$; 1.306)	1.5367 (6)–1.5655 (7)	1.546	–	4.93
O1	2				*2*	1.50
O2	1				*3*	1.26
O3	1				*3*	1.25
O4	1				*5*	1.17
O1*W*	2				–	0.47
O2*W*	2				–	0.43
O3*W*	3				–	0.53
O4*W*	3				–	0.48
O5*W*	3				–	0.49
O6*W*	2				*1*	0.36
O7*W*	2				–	0.43
$Na_3(PO_4)(H_2O)_6$						
Na1	5	Ψ-1 octahedron (4*mm*; 22.301)	2.3505 (6)–2.5944 (5)	2.418	3	0.98
Na2	6	twisted trigonal prism (32; 6.248)	2.3508 (5)–2.5269 (6)	2.428	6	1.08
Na3	6	twisted trigonal prism (32; 7.483)	2.3549 (5)–2.5365 (6)	2.433	5	1.07
Na4	6	trigonal antifrustum (3*m*; 12.318)	2.3115 (5)–2.9741 (6)	2.485	5	1.08
Na5	6	twisted trigonal prism (32; 6.907)	2.3151 (5)–2.5838 (6)	2.395	6	1.18
Na6	6	isosceles wedge (*mm*2; 22.202)	2.3321 (5)–2.9641 (5)	2.533	3	0.96
P1	4	tetrahedron ($\bar{4}3m$; 0.995)	1.5336 (5)–1.5525 (5)	1.544	–	4.92
P2	4	tetrahedron ($\bar{4}3m$; 0.823)	1.5348 (5)–1.5509 (5)	1.545	–	4.95
O1	3				*1*	1.69
O2	2				*3*	1.41
O3	3				*2*	1.54
O4	3				*1*	1.70
O5	1				*5*	1.21
O6	1				*3*	1.26
O7	1				*4*	1.22
O8	1				*4*	1.21
O1*W*	2				–	0.41
O2*W*	3				–	0.36
O3*W*	2				–	0.42
O4*W*	2				–	0.34
O5*W*	2				–	0.43
O6*W*	2				*1*	0.36
O7*W*	3				–	0.52
O8*W*	3				–	0.49
O9*W*	2				–	0.46
O10*W*	3				–	0.48
O11*W*	2				–	0.36
O12*W*	2				–	0.35

The description of the closest matching ideal coordination polyhedron for the three Na^+ sites and quantification of the distortion (δ) from it was performed with the *Polynator* program (Link & Niewa, 2023). In all cases, the idealized coordination polyhedron can be derived from a Bailar twist (dynamic) with moderate distortions (Table 2). The overall mean Na—O bond length in the three [NaO_6] polyhedra amounts to 2.415 Å, in good agreement with the literature value of 2.441 (112) Å averaged from 920 individual polyhedra (Gagné & Hawthorne, 2016).

The P—O distances in the orthophosphate group lie in a narrow range (Table 2) with a mean of 1.546 Å, again in good agreement with the literature value of 1.537 (39) Å averaged from 3650 phosphate tetrahedra (Gagné & Hawthorne, 2018). The slight angular distortions of the $[PO_4]^{3-}$ tetrahedron is seen by the variation of the O—P—O angles ranging from 108.28 (3) to 111.12 (4)°.

The crystal structure of $Na_3(PO_4)(H_2O)_7$ is consolidated by an intricate network of O—H···O hydrogen bonds between water molecules as donor groups and phosphate O atoms as acceptor atoms (Table 3, Fig. 4). All the water molecules contribute to the hydrogen bonding with two approximately linear O—H···O links. The number of hydrogen bonds accepted differs for the O atoms of the phosphate group. Atom O1, which is the only one additionally bound to Na^+, is the acceptor of two hydrogen bonds, O2 and O3 are each acceptors of three hydrogen bonds, while O4 is remarkably the acceptor of five hydrogen bonds. The $D\cdots A$ distances range from 2.5865 (9) to 3.2041 (11) Å, and on average can be classified as of medium strength (Jeffrey,

Table 3
Hydrogen-bond geometry (Å, °) for $Na_3(PO_4)(H_2O)_7$.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O4^{v}	0.84 (1)	2.09 (1)	2.9344 (9)	176 (2)
O1*W*—H1*WB*···O2^{iv}	0.85 (1)	1.74 (1)	2.5865 (9)	172 (2)
O2*W*—H2*WA*···O6*W*^{vi}	0.85 (1)	2.38 (1)	3.2042 (11)	163 (2)
O2*W*—H2*WB*···O4^{iv}	0.84 (1)	1.93 (1)	2.7634 (9)	175 (2)
O3*W*—H3*WA*···O1^{vii}	0.85 (1)	1.85 (1)	2.6867 (9)	168 (2)
O3*W*—H3*WB*···O3^{viii}	0.87 (1)	1.88 (1)	2.7391 (9)	172 (2)
O4*W*—H4*WA*···O2^{iv}	0.84 (1)	1.97 (1)	2.8058 (9)	173 (2)
O4*W*—H4*WB*···O3^{viii}	0.86 (1)	1.84 (1)	2.6978 (9)	171 (2)
O5*W*—H5*WA*···O3^{ix}	0.85 (1)	1.87 (1)	2.7114 (9)	173 (2)
O5*W*—H5*WB*···O4^{v}	0.85 (1)	1.92 (1)	2.7544 (9)	169 (2)
O6*W*—H6*WA*···O1^{ix}	0.85 (1)	1.99 (1)	2.8109 (9)	163 (2)
O6*W*—H6*WB*···O4^{vii}	0.84 (1)	2.01 (1)	2.8323 (9)	169 (2)
O7*W*—H7*WA*···O4^{viii}	0.85 (1)	2.02 (1)	2.8616 (9)	170 (2)
O7*W*—H7*WB*···O2^{ix}	0.86 (1)	1.93 (1)	2.7894 (9)	175 (2)

Symmetry codes: (iv) $x, y+1, z$; (v) $x-\frac{1}{2}, -y+1, z$; (vi) $-x+\frac{3}{2}, y, z-\frac{1}{2}$; (vii) $-x+\frac{3}{2}, y, z+\frac{1}{2}$; (viii) $-x+\frac{3}{2}, y+1, z+\frac{1}{2}$; (ix) $-x+1, -y+1, z+\frac{1}{2}$.

1997). It is noteworthy that only one hydrogen bond is formed with another water molecule as the acceptor (O6*W*), namely with the longest observed *D*···*A* distance (Table 3).

2.2. $Na_3(PO_4)(H_2O)_6$

$Na_3(PO_4)(H_2O)_6$ crystallizes in the triclinic space group $P\overline{1}$ and comprises two formula units in the asymmetric unit. The crystal structure consists of one fivefold coordinated Na^+ cation (Na1) and five sixfold coordinated Na^+ cations (Na2–Na6) with different idealized coordination polyhedra (Fig. 5, Tables 2 and 4). The mean Na—O distance of the fivefold coordinated Na^+ is 2.418 Å, in very good agreement with the literature value of 2.413 (108) Å (Gagné & Hawthorne, 2016). The total mean value of the Na—O distance of the five sixfold-coordinated Na^+ cations is 2.455 Å, which is slightly longer than in the heptahydrate and corresponds almost perfectly with the value given in the literature (see above).

The lower water content compared to $Na_3(PO_4)(H_2O)_7$ can be seen in a lower number of coordinating water molecules for the cations. Overall, only two of the six-coordinated cations (Na2, Na5) have all ligand atoms from water molecules, two cations (Na3, Na4) have five water molecules and one phosphate O atom in the coordination sphere, and one (Na6) has only three water molecules and three phosphate O atoms; the five-coordinated Na1 also has three water molecules as direct coordination partners. The individual polyhedra are in turn connected to each other by sharing corners and edges, with four of the water molecules (O2*W*, O7*W*, O8*W*, O10*W*) bound to three cations simultaneously and the rest bound to two (Table 2).

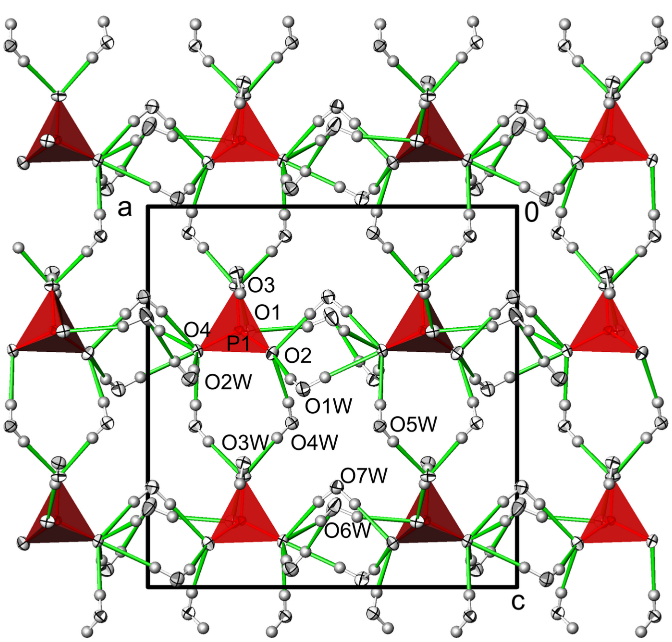


Figure 4
$Na_3(PO_4)(H_2O)_7$. Hydrogen-bonding network (green lines) between water molecules and phosphate tetrahedra. Displacement ellipsoids are as in Fig. 1.

Table 4
Selected bond lengths (Å) for $Na_3(PO_4)(H_2O)_6$.

Na1—O4	2.3205 (6)	Na4—O1	2.3278 (5)
Na1—O4^{i}	2.3722 (5)	Na4—O6*W*	2.3433 (5)
Na1—O4*W*	2.3907 (6)	Na4—O3*W*^{iii}	2.3463 (5)
Na1—O2*W*	2.4107 (6)	Na4—O7*W*	2.6079 (6)
Na1—O8*W*^{ii}	2.5944 (5)	Na4—O2*W*^{v}	2.9741 (6)
Na2—O5*W*	2.3508 (5)	Na5—O7*W*	2.3151 (5)
Na2—O1*W*	2.3690 (6)	Na5—O9*W*	2.3155 (5)
Na2—O3*W*	2.3726 (5)	Na5—O9*W*^{vi}	2.3577 (5)
Na2—O1*W*^{iii}	2.4245 (6)	Na5—O8*W*	2.3971 (5)
Na2—O12*W*^{iii}	2.5221 (6)	Na5—O10*W*	2.4006 (5)
Na2—O4*W*	2.5269 (6)	Na5—O2*W*^{v}	2.5838 (6)
Na3—O5*W*	2.3549 (5)	Na6—O3	2.3321 (5)
Na3—O1	2.3707 (5)	Na6—O12*W*	2.3913 (5)
Na3—O8*W*^{ii}	2.4357 (5)	Na6—O11*W*	2.4088 (5)
Na3—O11*W*^{iv}	2.4372 (5)	Na6—O2^{vii}	2.4443 (5)
Na3—O7*W*^{ii}	2.4623 (5)	Na6—O3^{vii}	2.6552 (6)
Na3—O6*W*	2.5365 (6)	Na6—O10*W*	2.9641 (5)
Na4—O10*W*	2.3115 (5)		

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+1, -y, -z$; (iv) $x-1, y, z$; (v) $x, y+1, z$; (vi) $-x+2, -y+2, -z+1$; (vii) $-x+2, -y+1, -z+1$.

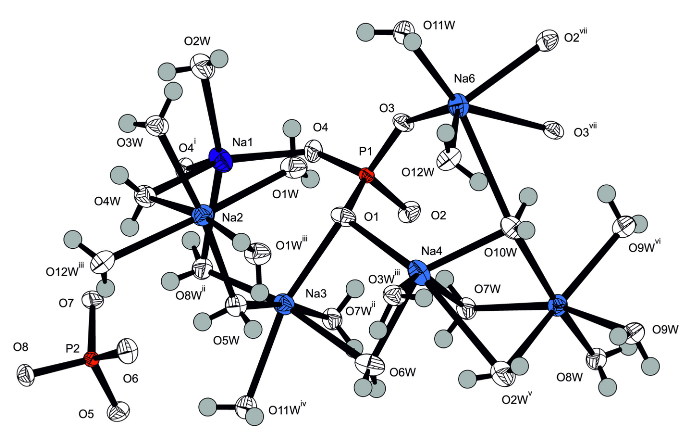


Figure 5
The asymmetric unit of $Na_3(PO_4)(H_2O)_6$ expanded to show the full coordination environments of the six Na^+ cations. Displacement ellipsoid are as in Fig. 1. Symmetry codes refer to Table 4.

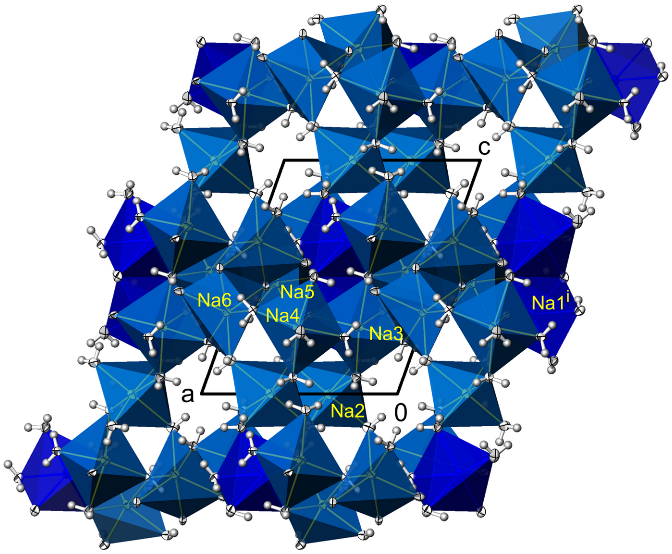


Figure 6
$Na_3(PO_4)(H_2O)_6$. Linkage of $[NaO_2(H_2O)_3]$ (Na1), $[Na(H_2O)_6]$ (Na2, Na5), $[NaO(H_2O)_5]$ (Na3, Na4), and $[NaO_3(H_2O)_3]$ (Na6) polyhedra into a framework structure in a view along $[0\bar{1}0]$. Displacement ellipsoids are as in Fig. 1. [Symmetry code: (i) $1 - x, y, z$.]

Another difference to $Na_3(PO_4)(H_2O)_7$ concerns the resulting linkage of these polyhedra, which in this case is not in the form of layers but as a three-dimensional framework structure (Fig. 6). The $[PO_4]^{3-}$ tetrahedra are isolated and located in the voids of this arrangement (Fig. 7). It is noteworthy here that the two unique $[PO_4]^{3-}$ tetrahedra exhibit different properties. While all the O atoms of one tetrahedron (P1) are also shared with Na^+ cations, the O atoms of the other tetrahedron (P2) belong exclusively to the P atom. However, these differences are not noticeable in the P—O bond lengths (Table 2). The range of P—O bond lengths is approximately the same in both phosphate tetrahedra, and the respective mean values correspond to the literature value (see above). The range of O—P—O angles also does not differ significantly, ranging from 107.68 (3) to 110.03 (2)° for P1 and from 108.71 (3) to 110.23 (2)° for P2.

A network of O—H⋯O hydrogen bonds consolidates the crystal structure of the hexahydrate and exhibit similar $D\cdots A$ distances and angles (Table 5, Fig. 8) as the heptahydrate. With only one water molecule as an additional acceptor (O6*W*), the

Table 5
Hydrogen-bond geometry (Å, °) for $Na_3(PO_4)(H_2O)_6$.

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1*W*—H1*WA*⋯O1	0.85 (1)	1.83 (1)	2.6704 (7)	171 (1)
O1*W*—H1*WB*⋯O5^{viii}	0.86 (1)	2.09 (1)	2.9417 (6)	172 (1)
O2*W*—H2*WA*⋯O6*W*^{ix}	0.82 (1)	2.47 (1)	3.1079 (8)	136 (1)
O2*W*—H2*WB*⋯O5^{viii}	0.82 (1)	2.03 (1)	2.8343 (7)	167 (1)
O3*W*—H3*WA*⋯O8^{x}	0.83 (1)	1.84 (1)	2.6651 (6)	175 (1)
O3*W*—H3*WB*⋯O8^{viii}	0.85 (1)	2.03 (1)	2.8469 (6)	161 (1)
O4*W*—H4*WA*⋯O7	0.82 (1)	2.04 (1)	2.8552 (6)	173 (1)
O4*W*—H4*WB*⋯O8^{x}	0.81 (1)	2.00 (1)	2.7987 (7)	170 (1)
O5*W*—H5*WA*⋯O6	0.84 (1)	1.80 (1)	2.6359 (7)	172 (1)
O5*W*—H5*WB*⋯O5^{xi}	0.83 (1)	2.43 (1)	3.2184 (7)	159 (1)
O6*W*—H6*WA*⋯O8^{xi}	0.84 (1)	1.95 (1)	2.7557 (6)	159 (1)
O6*W*—H6*WB*⋯O2^{ii}	0.84 (1)	1.84 (1)	2.6508 (6)	160 (1)
O7*W*—H7*WA*⋯O2	0.86 (1)	1.77 (1)	2.6209 (6)	172 (1)
O7*W*—H7*WB*⋯O2^{ii}	0.85 (1)	2.12 (1)	2.9658 (6)	174 (1)
O8*W*—H8*WA*⋯O7^{ii}	0.83 (1)	1.95 (1)	2.7783 (7)	172 (1)
O8*W*—H8*WB*⋯O4^{v}	0.84 (1)	1.81 (1)	2.6220 (6)	164 (1)
O9*W*—H9*WA*⋯O5^{xii}	0.82 (1)	1.93 (1)	2.7531 (7)	174 (1)
O9*W*—H9*WB*⋯O3^{v}	0.84 (1)	1.90 (1)	2.7235 (6)	167 (1)
O10*W*—H10*A*⋯O7^{xii}	0.83 (1)	1.91 (1)	2.7345 (6)	175 (1)
O10*W*—H10*B*⋯O3^{vii}	0.85 (1)	1.85 (1)	2.6902 (6)	171 (1)
O11*W*—H11*A*⋯O6^{iii}	0.87 (1)	1.90 (1)	2.7666 (6)	173 (1)
O11*W*—H11*B*⋯O5^{viii}	0.85 (1)	2.00 (1)	2.8460 (7)	176 (1)
O12*W*—H12*A*⋯O6^{iii}	0.86 (1)	1.90 (1)	2.7438 (7)	168 (1)
O12*W*—H12*B*⋯O7^{xii}	0.85 (1)	1.97 (1)	2.8165 (6)	171 (1)

Symmetry codes: (ii) $-x+1, -y+1, -z+1$; (iii) $-x+1, -y, -z$; (v) $x, y+1, z$; (vii) $-x+2, -y+1, -z+1$; (viii) $x+1, y, z$; (ix) $x, y-1, z$; (x) $-x, -y-1, -z$; (xi) $-x, -y, -z$; (xii) $x+1, y+1, z$.

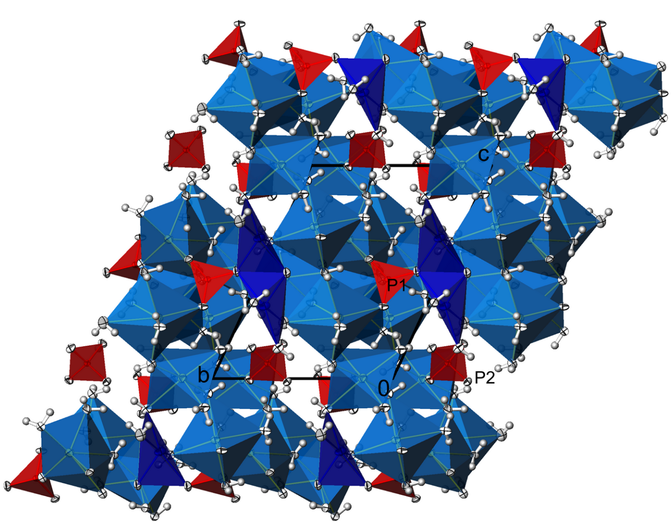


Figure 7
$Na_3(PO_4)(H_2O)_6$. View of the crystal structure along $[\bar{1}00]$ showing the $[PO_4]^{3-}$ tetrahedra in the voids of the cationic framework. Displacement ellipsoids are as in Fig. 1.

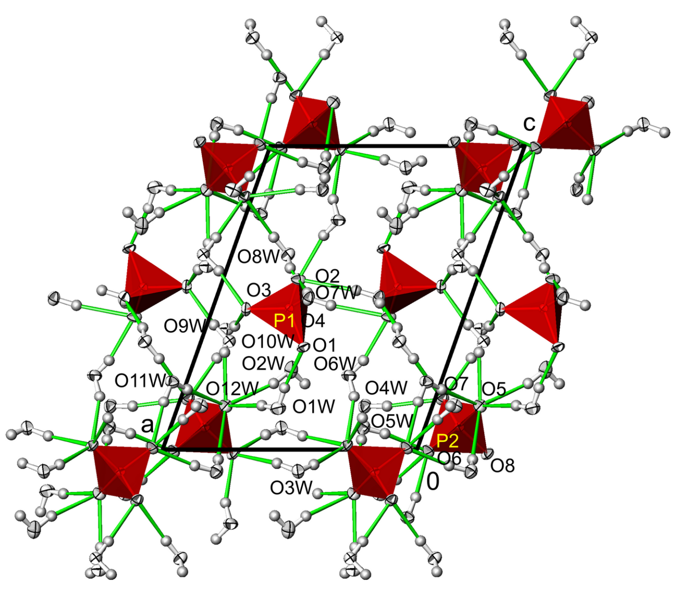


Figure 8
$Na_3(PO_4)(H_2O)_6$. Hydrogen-bonding network (green lines) between water molecules and phosphate tetrahedra. Displacement ellipsoids are as in Fig. 1.

Table 6
Experimental details.

	$Na_3(PO_4)(H_2O)_7$	$Na_3(PO_4)(H_2O)_6$
Crystal data		
M_r	290.05	272.04
Crystal system, space group	Orthorhombic, $Pca2_1$	Triclinic, $P\bar{1}$
Temperature (K)	100	100
a, b, c (Å)	12.3169 (7), 6.5324 (3), 12.6602 (7)	9.5490 (4), 9.6353 (5), 12.1401 (6)
α, β, γ (°)	90, 90, 90	109.289 (4), 101.228 (4), 108.476 (4)
V (Å^3)	1018.63 (9)	942.35 (8)
Z	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.44	0.46
Crystal size (mm)	0.28 × 0.19 × 0.10	0.13 × 0.09 × 0.04
Data collection		
Diffractometer	Bruker APEXII CCD	Stoe STADIVARI
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)	Multi-scan (*LANA*; Koziskova *et al.*, 2016)
T_{min}, T_{max}	0.695, 0.748	0.911, 0.991
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	44325, 6462, 6108	42672, 9215, 8427
R_{int}	0.032	0.018
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.020, 0.046, 1.07	0.020, 0.056, 1.06
No. of reflections	6462	9215
No. of parameters	192	325
No. of restraints	15	24
H-atom treatment	All H-atom parameters refined	Only H-atom coordinates refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.32, −0.22	0.53, −0.32
Absolute structure	Flack x determined using 2767 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)	–
Absolute structure parameter	0.00 (3)	–

Computer programs: *APEX3* and *SAINT* (Bruker, 2021), *X-AREA* (Stoe, 2024), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *ATOMS* (Dowty, 2006) and *publCIF* (Westrip, 2010).

phosphate O atoms primarily assume this role in the hexahydrate as well. The differences between the two phosphate groups are clearly evident in the hydrogen-bonding network. The total number of accepted hydrogen bonds of seven for the P1 phosphate tetrahedron (which also bonds to sodium ions) is significantly lower than for the 'free' P2 tetrahedron with 15.

2.3. Bond valence sum calculation

Calculations of bond-valence sums (BVS; Brown, 2002) were performed with the program *ECoN21* (Ilinca, 2022) without contributions of H atoms. The BVS values of all atomic sites are listed in Table 2 and correspond to expectations for Na (1.0 valence unit, v. u.) and for P (5.0 v. u.). The BVS values obtained for the O atoms reflect their roles in the hydrogen-bonding networks. All water O atoms (O*W) have a value of less than 0.5 v.u., and all phosphate O atoms have a value significantly below the expected BVS value of 2.0 v.u., which is due to their role as acceptors of hydrogen bonds. There is a consistent trend for these phosphate O atoms showing that the BVS value decreases as the number of accepted hydrogen bonds increases (Tables 2, 3 and 5).

3. Database survey

A search of the Inorganic Crystal Structure Database (ICSD; data release 2025-1; Zagorac *et al.*, 2019) for $Na_3(XO_4)(H_2O)_n$ phases with tetrahedral $(XO_4)^{3-}$ anions (X = P, As, V) revealed two entries for orthophosphates, $Na_3(PO_4)(H_2O)_8$ (Larbot & Durand, 1983) and $Na_3(PO_4)(H_2O)_{0.5}$ (Averbuch-Pouchot & Durif, 1983), no entry for orthoarsenates, and one entry for orthovanadates, $Na_3(VO_4)(H_2O)_3$ (Kato & Takayama-Muromachi, 1987).

$Na_3(PO_4)(H_2O)_8$ (space group $P\bar{1}$) comprises two formula units in the asymmetric unit. From the six octahedrally surrounded Na^+ cations, five exhibit solely water molecules in the coordination sphere, and one four water molecules and two O atoms from phosphate groups. Like in $Na_3(PO_4)(H_2O)_7$, the polyhedra around the Na^+ cations are linked into a layered arrangement, with $[PO_4]^{3-}$ groups situated in between. Hydrogen atoms have not been determined for this structure, hence details on hydrogen-bonding interactions are limited to $D\cdots A$ distances.

$Na_3(PO_4)(H_2O)_{0.5}$ (space group $C2/c$) comprises one formula unit in the asymmetric unit. One of the three octahedrally surrounded Na^+ cations has solely phosphate O atoms in the coordination sphere, while the other two have one water molecule and five phosphate O atoms as ligands. Linking these polyhedra leads a framework structure. The water molecule is situated on a twofold rotation axis and is the donor of two symmetry-related hydrogen bonds of medium strength.

$Na_3(VO_4)(H_2O)_3$ (space group $R3$) comprises one third of the formula unit in the asymmetric unit, with the V and one O atom situated on a threefold rotation axis. The $[NaO_3(H_2O)_3]$ octahedron shares its edges with neighbouring octahedra to form a framework structure. In this structure, too, two hydrogen bonds of medium strength are formed by the water molecule.

4. Synthesis and crystallization

For the crystal growth of $Na_3(PO_4)(H_2O)_7$, a concentrated aqueous solution of $Na_3(PO_4)$ was prepared in a polypropylene beaker from commercially available $Na_3(PO_4)(H_2O)_6$ (Budenheim KG, Germany) and evaporated for one day at 361 K in a drying oven. Pieces were broken off from the compact product and crushed again by gentle pressing between two glass slides. Crystals were isolated under a polarizing microscope and tested on a single crystal diffractometer. Besides weakly diffracting multi-domain crystals of undetermined composition, high-quality crystals of $Na_3(PO_4)(H_2O)_7$ were obtained this way.

A suitable single crystals of $Na_3(PO_4)(H_2O)_6$ was taken directly from the storage container of a commercially available sample (Budenheim KG, Germany).

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 6. To prevent possible water release, data collections were performed at 100 K. Experience has shown that measurements at low temperatures also enable better localization of hydrogen atom positions from difference-Fourier maps, which was the case for all hydrogen atoms in both hydrate phases. Their O—H bond lengths were refined with restraints using a value of 0.85 (1) Å. Quick measurements of crystals of both compounds at room temperature showed no notable differences from the low-temperature measurements.

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supporting information

Acta Cryst. (2025). E**81**, 1119-1125 [https://doi.org/10.1107/S2056989025009843]

The missing representatives of the hydrated sodium orthophosphate phases: $Na_3(PO_4)(H_2O)_7$ and $Na_3(PO_4)(H_2O)_6$

Matthias Weil and Berthold Söger

Computing details

Trisodium orthophosphate hexahydrate (Na3PO4H2O6)

Crystal data

$Na_3(PO_4)(H_2O)_6$	$Z = 4$
$M_r = 272.04$	$F(000) = 560$
Triclinic, $P\overline{1}$	$D_x = 1.917$ Mg m^{-3}
$a = 9.5490$ (4) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 9.6353$ (5) Å	Cell parameters from 42515 reflections
$c = 12.1401$ (6) Å	$\theta = 1.9–36.7°$
$\alpha = 109.289$ (4)°	$\mu = 0.46$ mm^{-1}
$\beta = 101.228$ (4)°	$T = 100$ K
$\gamma = 108.476$ (4)°	Plate, colourless
$V = 942.35$ (8) Å^3	0.13 × 0.09 × 0.04 mm

Data collection

Stoe STADIVARI diffractometer	42672 measured reflections
Radiation source: Axo_Mo	9215 independent reflections
Graded multilayer mirror monochromator	8427 reflections with $I > 2\sigma(I)$
Detector resolution: 13.33 pixels mm^{-1}	$R_{int} = 0.018$
rotation method, ω scans	$\theta_{max} = 36.9°$, $\theta_{min} = 2.4°$
Absorption correction: multi-scan (*LANA*; Koziskova *et al.*, 2016)	$h = -16 \rightarrow 13$
$T_{min} = 0.911$, $T_{max} = 0.991$	$k = -10 \rightarrow 16$
	$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	Primary atom site location: dual
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.020$	Only H-atom coordinates refined
$wR(F^2) = 0.056$	$w = 1/[\sigma^2(F_o^2) + (0.0291P)^2 + 0.1762P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.002$
9215 reflections	$\Delta\rho_{max} = 0.53$ e Å^{-3}
325 parameters	$\Delta\rho_{min} = -0.32$ e Å^{-3}
24 restraints	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Na1	0.46040 (3)	−0.10173 (3)	0.34021 (2)	0.01131 (5)
Na2	0.35186 (3)	−0.16635 (3)	−0.00188 (2)	0.00949 (5)
Na3	0.31635 (3)	0.17465 (3)	0.28593 (2)	0.00889 (4)
Na4	0.63254 (3)	0.45792 (3)	0.28635 (2)	0.01083 (5)
Na5	0.81993 (3)	0.85412 (3)	0.47425 (2)	0.00871 (4)
Na6	1.01416 (3)	0.39929 (3)	0.34657 (2)	0.00953 (5)
P1	0.69885 (2)	0.28053 (2)	0.46564 (2)	0.00492 (3)
P2	−0.13497 (2)	−0.26690 (2)	0.07362 (2)	0.00497 (3)
O1	0.58849 (5)	0.23882 (5)	0.33732 (4)	0.00922 (7)
O2	0.70340 (5)	0.43730 (5)	0.56120 (4)	0.00895 (7)
O3	0.86741 (5)	0.31380 (5)	0.46279 (4)	0.00820 (7)
O4	0.63891 (5)	0.14101 (5)	0.50280 (4)	0.00914 (7)
O5	−0.18726 (5)	−0.13720 (5)	0.14385 (4)	0.00937 (7)
O6	−0.04459 (5)	−0.20890 (5)	−0.00562 (4)	0.00942 (7)
O7	−0.03024 (5)	−0.30105 (5)	0.16635 (4)	0.00814 (7)
O8	−0.28289 (5)	−0.42346 (5)	−0.01384 (4)	0.00825 (7)
O1W	0.60359 (5)	0.02983 (6)	0.13572 (4)	0.01135 (7)
H1WA	0.6072 (14)	0.0949 (13)	0.2043 (10)	0.017*
H1WB	0.6714 (13)	−0.0106 (14)	0.1449 (11)	0.017*
O2W	0.60598 (6)	−0.25279 (6)	0.26337 (5)	0.01358 (8)
H2WA	0.5326 (13)	−0.3403 (13)	0.2176 (11)	0.020*
H2WB	0.6559 (14)	−0.2320 (15)	0.2186 (11)	0.020*
O3W	0.43736 (5)	−0.37555 (5)	−0.07135 (4)	0.00970 (7)
H3WA	0.3845 (13)	−0.4408 (13)	−0.0491 (10)	0.015*
H3WB	0.5313 (12)	−0.3654 (13)	−0.0451 (10)	0.015*
O4W	0.26544 (5)	−0.28566 (6)	0.14281 (4)	0.01040 (7)
H4WA	0.1781 (12)	−0.2915 (14)	0.1430 (10)	0.016*
H4WB	0.2588 (13)	−0.3752 (13)	0.1040 (10)	0.016*
O5W	0.24137 (5)	0.01652 (5)	0.07208 (4)	0.01034 (7)
H5WA	0.1484 (12)	−0.0496 (13)	0.0527 (10)	0.016*
H5WB	0.2323 (13)	0.0709 (13)	0.0327 (10)	0.016*
O6W	0.37090 (5)	0.42450 (6)	0.24429 (4)	0.01154 (8)
H6WA	0.3214 (13)	0.4155 (14)	0.1753 (10)	0.017*
H6WB	0.3349 (13)	0.4744 (14)	0.2944 (10)	0.017*
O7W	0.63802 (5)	0.65073 (5)	0.49826 (4)	0.00930 (7)
H7WA	0.6496 (13)	0.5753 (13)	0.5170 (10)	0.014*
H7WB	0.5398 (12)	0.6220 (13)	0.4755 (10)	0.014*
O8W	0.77912 (5)	1.03439 (5)	0.64277 (4)	0.00946 (7)
H8WA	0.8590 (12)	1.1091 (13)	0.6996 (10)	0.014*

H8WB	0.7518 (13)	1.0782 (13)	0.5982 (10)	0.014*
O9W	0.91801 (5)	1.03959 (5)	0.39645 (4)	0.00958 (7)
H9WA	0.8919 (13)	0.9917 (13)	0.3208 (9)	0.014*
H9WB	0.8890 (13)	1.1149 (13)	0.4071 (10)	0.014*
O10W	0.88846 (5)	0.64630 (6)	0.35754 (4)	0.00997 (7)
H10A	0.9146 (13)	0.6684 (13)	0.3019 (10)	0.015*
H10B	0.9719 (12)	0.6652 (13)	0.4111 (10)	0.015*
O11W	1.05705 (5)	0.17297 (5)	0.22373 (4)	0.00941 (7)
H11A	1.0618 (13)	0.1875 (13)	0.1572 (10)	0.014*
H11B	0.9869 (12)	0.0787 (12)	0.1988 (10)	0.014*
O12W	0.91400 (6)	0.38437 (6)	0.14452 (4)	0.01083 (7)
H12A	0.9607 (13)	0.3419 (13)	0.0989 (10)	0.016*
H12B	0.9286 (13)	0.4756 (12)	0.1426 (11)	0.016*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.00846 (10)	0.01261 (11)	0.00943 (11)	0.00320 (9)	0.00247 (8)	0.00208 (9)
Na2	0.00993 (10)	0.00898 (10)	0.00958 (10)	0.00441 (8)	0.00319 (8)	0.00350 (8)
Na3	0.00822 (10)	0.00915 (10)	0.00819 (10)	0.00328 (8)	0.00196 (8)	0.00311 (8)
Na4	0.00839 (10)	0.01256 (11)	0.00898 (10)	0.00200 (9)	0.00190 (8)	0.00434 (9)
Na5	0.00863 (10)	0.00774 (10)	0.00979 (10)	0.00296 (8)	0.00392 (8)	0.00363 (8)
Na6	0.00947 (10)	0.00953 (10)	0.00881 (10)	0.00287 (8)	0.00378 (8)	0.00354 (8)
P1	0.00444 (5)	0.00515 (5)	0.00481 (5)	0.00190 (4)	0.00119 (4)	0.00196 (4)
P2	0.00499 (5)	0.00510 (5)	0.00470 (5)	0.00206 (4)	0.00134 (4)	0.00208 (4)
O1	0.00815 (16)	0.01242 (18)	0.00564 (15)	0.00500 (14)	0.00015 (13)	0.00263 (14)
O2	0.01142 (17)	0.00766 (16)	0.00709 (16)	0.00488 (14)	0.00300 (13)	0.00145 (13)
O3	0.00551 (14)	0.01020 (16)	0.01047 (17)	0.00352 (13)	0.00329 (13)	0.00557 (14)
O4	0.00861 (16)	0.00780 (16)	0.01155 (17)	0.00204 (13)	0.00348 (14)	0.00591 (14)
O5	0.00990 (16)	0.00825 (16)	0.00981 (17)	0.00520 (14)	0.00346 (14)	0.00214 (14)
O6	0.00998 (16)	0.01025 (17)	0.00833 (16)	0.00251 (14)	0.00420 (13)	0.00521 (14)
O7	0.00774 (15)	0.00951 (16)	0.00773 (16)	0.00397 (13)	0.00111 (13)	0.00471 (14)
O8	0.00684 (15)	0.00686 (15)	0.00772 (16)	0.00093 (13)	0.00056 (13)	0.00209 (13)
O1W	0.01197 (18)	0.01287 (18)	0.00871 (17)	0.00664 (15)	0.00221 (14)	0.00321 (15)
O2W	0.00987 (17)	0.0143 (2)	0.0168 (2)	0.00397 (15)	0.00499 (16)	0.00754 (17)
O3W	0.00861 (16)	0.01147 (18)	0.01137 (17)	0.00478 (14)	0.00439 (14)	0.00633 (15)
O4W	0.00843 (16)	0.00966 (17)	0.01095 (17)	0.00372 (14)	0.00291 (14)	0.00203 (14)
O5W	0.00952 (16)	0.00937 (17)	0.01091 (17)	0.00374 (14)	0.00255 (14)	0.00350 (14)
O6W	0.01125 (17)	0.0173 (2)	0.00671 (16)	0.00813 (16)	0.00269 (14)	0.00377 (15)
O7W	0.00787 (16)	0.00895 (16)	0.01092 (17)	0.00252 (13)	0.00286 (13)	0.00505 (14)
O8W	0.00934 (16)	0.00804 (16)	0.00966 (17)	0.00319 (14)	0.00179 (14)	0.00334 (14)
O9W	0.01174 (17)	0.00927 (17)	0.00822 (17)	0.00525 (14)	0.00296 (14)	0.00359 (14)
O10W	0.00814 (16)	0.01246 (18)	0.00823 (16)	0.00333 (14)	0.00267 (13)	0.00402 (14)
O11W	0.01033 (16)	0.00900 (17)	0.00891 (16)	0.00350 (14)	0.00338 (14)	0.00413 (14)
O12W	0.01409 (18)	0.00960 (17)	0.01098 (18)	0.00646 (15)	0.00509 (15)	0.00482 (14)

Geometric parameters (Å, º)

Na1—O4	2.3205 (6)	Na4—O2W^{v}	2.9741 (6)
Na1—O4^{i}	2.3722 (5)	Na5—O7W	2.3151 (5)
Na1—O4W	2.3907 (6)	Na5—O9W	2.3155 (5)
Na1—O2W	2.4107 (6)	Na5—O9W^{vi}	2.3577 (5)
Na1—O8W^{ii}	2.5944 (5)	Na5—O8W	2.3971 (5)
Na2—O5W	2.3508 (5)	Na5—O10W	2.4006 (5)
Na2—O1W	2.3690 (6)	Na5—O2W^{v}	2.5838 (6)
Na2—O3W	2.3726 (5)	Na6—O3	2.3321 (5)
Na2—O1W^{iii}	2.4245 (6)	Na6—O12W	2.3913 (5)
Na2—O12W^{iii}	2.5221 (6)	Na6—O11W	2.4088 (5)
Na2—O4W	2.5269 (6)	Na6—O2^{vii}	2.4443 (5)
Na3—O5W	2.3549 (5)	Na6—O3^{vii}	2.6552 (6)
Na3—O1	2.3707 (5)	Na6—O10W	2.9641 (5)
Na3—O8W^{ii}	2.4357 (5)	P1—O4	1.5336 (5)
Na3—O11W^{iv}	2.4372 (5)	P1—O1	1.5419 (4)
Na3—O7W^{ii}	2.4623 (5)	P1—O3	1.5482 (4)
Na3—O6W	2.5365 (6)	P1—O2	1.5525 (5)
Na4—O10W	2.3115 (5)	P2—O6	1.5348 (5)
Na4—O1	2.3278 (5)	P2—O7	1.5462 (4)
Na4—O6W	2.3433 (5)	P2—O5	1.5476 (4)
Na4—O3W^{iii}	2.3463 (5)	P2—O8	1.5509 (5)
Na4—O7W	2.6079 (6)		
O1—P1—O2	108.70 (2)	P1—O2—Na6^{vii}	100.64 (2)
O1—P1—O3	110.03 (2)	P1—O3—Na6	136.44 (3)
O3—P1—O2	107.68 (3)	P1—O3—Na6^{vii}	92.37 (2)
O4—P1—O1	109.62 (3)	Na6—O3—Na6^{vii}	95.452 (17)
O4—P1—O2	110.25 (3)	P1—O4—Na1^{i}	136.46 (3)
O4—P1—O3	110.52 (2)	P1—O4—Na1	114.59 (3)
O5—P2—O8	108.71 (2)	Na1—O4—Na1^{i}	97.030 (18)
O6—P2—O5	109.77 (3)	Na2—O1W—Na2^{iii}	94.480 (19)
O6—P2—O7	109.83 (2)	Na2—O1W—H1WA	116.4 (8)
O6—P2—O8	108.30 (2)	Na2^{iii}—O1W—H1WA	109.8 (8)
O7—P2—O5	110.23 (2)	Na2^{iii}—O1W—H1WB	109.4 (8)
O7—P2—O8	109.96 (2)	Na2—O1W—H1WB	113.0 (8)
O4—Na1—O4^{i}	82.970 (18)	H1WA—O1W—H1WB	112.2 (11)
O4—Na1—O2W	107.43 (2)	Na1—O2W—Na4^{viii}	131.39 (2)
O4^{i}—Na1—O2W	118.22 (2)	Na1—O2W—Na5^{viii}	96.15 (2)
O4—Na1—O4W	159.42 (2)	Na1—O2W—H2WA	99.2 (8)
O4^{i}—Na1—O4W	108.745 (19)	Na1—O2W—H2WB	121.8 (8)
O4—Na1—O8W^{ii}	93.816 (18)	Na4^{viii}—O2W—H2WA	63.3 (8)
O4^{i}—Na1—O8W^{ii}	63.542 (16)	Na4^{viii}—O2W—H2WB	106.7 (8)
O4W—Na1—O2W	82.410 (19)	Na5^{viii}—O2W—Na4^{viii}	74.081 (16)
O4W—Na1—O8W^{ii}	77.394 (17)	Na5^{viii}—O2W—H2WA	134.0 (8)
O1W—Na2—O1W^{iii}	85.520 (19)	Na5^{viii}—O2W—H2WB	103.7 (9)
O1W—Na2—O3W	94.509 (18)	H2WA—O2W—H2WB	104.3 (12)

O1W^{iii}—Na2—O4W	168.587 (19)	Na2—O3W—H3WA	100.2 (8)
O1W—Na2—O4W	98.343 (18)	Na2—O3W—H3WB	124.6 (7)
O1W^{iii}—Na2—O12W^{iii}	96.788 (18)	Na4^{iii}—O3W—Na2	104.369 (19)
O1W—Na2—O12W^{iii}	177.322 (19)	Na4^{iii}—O3W—H3WA	115.0 (8)
O3W—Na2—O1W^{iii}	103.980 (19)	Na4^{iii}—O3W—H3WB	107.3 (8)
O3W—Na2—O12W^{iii}	83.629 (18)	H3WA—O3W—H3WB	105.8 (11)
O5W—Na2—O1W^{iii}	82.339 (18)	Na1—O4W—Na2	103.47 (2)
O5W—Na2—O1W	90.266 (19)	Na1—O4W—H4WA	111.4 (8)
O5W—Na2—O3W	172.34 (2)	Na1—O4W—H4WB	123.6 (8)
O5W—Na2—O4W	86.890 (18)	Na2—O4W—H4WA	111.5 (8)
O5W—Na2—O12W^{iii}	91.388 (18)	Na2—O4W—H4WB	96.6 (8)
O1—Na3—O6W	87.697 (18)	H4WA—O4W—H4WB	108.8 (11)
O1—Na3—O7W^{ii}	89.260 (18)	Na2—O5W—Na3	120.57 (2)
O1—Na3—O8W^{ii}	103.275 (18)	Na2—O5W—H5WA	99.2 (8)
O1—Na3—O11W^{iv}	164.843 (19)	Na2—O5W—H5WB	115.8 (8)
O5W—Na3—O1	98.056 (19)	Na3—O5W—H5WA	104.6 (8)
O5W—Na3—O6W	89.307 (18)	Na3—O5W—H5WB	110.4 (8)
O5W—Na3—O7W^{ii}	171.710 (19)	H5WA—O5W—H5WB	103.3 (11)
O5W—Na3—O8W^{ii}	100.594 (19)	Na3—O6W—H6WA	119.0 (8)
O5W—Na3—O11W^{iv}	81.906 (18)	Na3—O6W—H6WB	99.5 (8)
O7W^{ii}—Na3—O6W	87.087 (18)	Na4—O6W—Na3	87.121 (18)
O8W^{ii}—Na3—O6W	163.889 (19)	Na4—O6W—H6WA	119.3 (8)
O8W^{ii}—Na3—O7W^{ii}	81.375 (17)	Na4—O6W—H6WB	125.4 (8)
O8W^{ii}—Na3—O11W^{iv}	91.578 (17)	H6WA—O6W—H6WB	104.4 (11)
O11W^{iv}—Na3—O6W	77.146 (17)	Na3^{ii}—O7W—Na4	169.88 (2)
O11W^{iv}—Na3—O7W^{ii}	90.011 (18)	Na3^{ii}—O7W—H7WA	93.0 (7)
O1—Na4—O2W^{v}	159.988 (18)	Na3^{ii}—O7W—H7WB	94.6 (7)
O1—Na4—O3W^{iii}	111.510 (19)	Na4—O7W—H7WA	80.0 (7)
O1—Na4—O6W	93.473 (19)	Na4—O7W—H7WB	94.1 (8)
O1—Na4—O7W	94.255 (18)	Na5—O7W—Na3^{ii}	93.036 (19)
O3W^{iii}—Na4—O2W^{v}	78.629 (17)	Na5—O7W—Na4	85.941 (18)
O3W^{iii}—Na4—O7W	147.855 (19)	Na5—O7W—H7WA	129.0 (7)
O6W—Na4—O2W^{v}	70.391 (18)	Na5—O7W—H7WB	126.4 (7)
O6W—Na4—O3W^{iii}	81.508 (18)	H7WA—O7W—H7WB	103.5 (10)
O6W—Na4—O7W	77.934 (18)	Na1^{ii}—O8W—H8WA	108.7 (8)
O7W—Na4—O2W^{v}	71.332 (16)	Na1^{ii}—O8W—H8WB	63.4 (8)
O10W—Na4—O1	116.965 (19)	Na3^{ii}—O8W—Na1^{ii}	89.467 (17)
O10W—Na4—O2W^{v}	75.406 (17)	Na3^{ii}—O8W—H8WA	107.3 (8)
O10W—Na4—O3W^{iii}	102.604 (19)	Na3^{ii}—O8W—H8WB	144.2 (8)
O10W—Na4—O6W	144.02 (2)	Na5—O8W—Na1^{ii}	131.86 (2)
O10W—Na4—O7W	80.946 (18)	Na5—O8W—Na3^{ii}	91.707 (18)
O7W—Na5—O2W^{v}	83.498 (18)	Na5—O8W—H8WA	116.7 (8)
O7W—Na5—O8W	85.300 (18)	Na5—O8W—H8WB	90.3 (8)
O7W—Na5—O9W	158.71 (2)	H8WA—O8W—H8WB	103.5 (11)
O7W—Na5—O9W^{vi}	116.928 (19)	Na5—O9W—Na5^{vi}	95.644 (19)
O7W—Na5—O10W	85.482 (18)	Na5^{vi}—O9W—H9WA	121.6 (8)
O8W—Na5—O2W^{v}	113.288 (19)	Na5—O9W—H9WA	108.6 (8)
O8W—Na5—O10W	161.013 (19)	Na5^{vi}—O9W—H9WB	108.7 (8)

O9W^{vi}—Na5—O2W^{v}	153.12 (2)	Na5—O9W—H9WB	118.8 (8)
O9W—Na5—O2W^{v}	76.393 (18)	H9WA—O9W—H9WB	104.4 (11)
O9W—Na5—O8W	96.191 (19)	Na4—O10W—Na5	91.035 (19)
O9W^{vi}—Na5—O8W	87.022 (18)	Na4—O10W—Na6	92.274 (18)
O9W—Na5—O9W^{vi}	84.355 (19)	Na4—O10W—H10A	112.3 (8)
O9W—Na5—O10W	98.413 (19)	Na4—O10W—H10B	133.7 (8)
O9W^{vi}—Na5—O10W	82.422 (18)	Na5—O10W—Na6	149.66 (2)
O2^{vii}—Na6—O3^{vii}	58.627 (15)	Na5—O10W—H10A	108.0 (8)
O2^{vii}—Na6—O10W	102.222 (17)	Na5—O10W—H10B	100.1 (8)
O3—Na6—O2^{vii}	121.259 (19)	Na6—O10W—H10A	98.6 (8)
O3—Na6—O3^{vii}	84.548 (17)	Na6—O10W—H10B	57.3 (7)
O3—Na6—O10W	90.449 (16)	H10A—O10W—H10B	106.6 (11)
O3^{vii}—Na6—O10W	56.888 (14)	Na3^{ix}—O11W—H11A	96.8 (7)
O3—Na6—O11W	107.102 (19)	Na3^{ix}—O11W—H11B	110.2 (7)
O3—Na6—O12W	126.569 (19)	Na6—O11W—Na3^{ix}	118.18 (2)
O11W—Na6—O2^{vii}	90.615 (18)	Na6—O11W—H11A	103.7 (7)
O11W—Na6—O3^{vii}	147.954 (18)	Na6—O11W—H11B	118.6 (8)
O11W—Na6—O10W	148.828 (18)	H11A—O11W—H11B	105.8 (10)
O12W—Na6—O2^{vii}	111.333 (19)	Na2^{iii}—O12W—H12A	92.3 (8)
O12W—Na6—O3^{vii}	117.639 (18)	Na2^{iii}—O12W—H12B	112.9 (8)
O12W—Na6—O10W	69.070 (16)	Na6—O12W—Na2^{iii}	118.81 (2)
O12W—Na6—O11W	79.823 (17)	Na6—O12W—H12A	108.2 (8)
P1—O1—Na3	125.14 (3)	Na6—O12W—H12B	114.4 (8)
P1—O1—Na4	113.58 (3)	H12A—O12W—H12B	107.1 (11)
Na4—O1—Na3	91.501 (18)		

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*+1, −*y*, −*z*; (iv) *x*−1, *y*, *z*; (v) *x*, *y*+1, *z*; (vi) −*x*+2, −*y*+2, −*z*+1; (vii) −*x*+2, −*y*+1, −*z*+1; (viii) *x*, *y*−1, *z*; (ix) *x*+1, *y*, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O1	0.85 (1)	1.83 (1)	2.6704 (7)	171 (1)
O1*W*—H1*WB*···O5^{ix}	0.86 (1)	2.09 (1)	2.9417 (6)	172 (1)
O2*W*—H2*WA*···O6*W*^{viii}	0.82 (1)	2.47 (1)	3.1079 (8)	136 (1)
O2*W*—H2*WB*···O5^{ix}	0.82 (1)	2.03 (1)	2.8343 (7)	167 (1)
O3*W*—H3*WA*···O8^{x}	0.83 (1)	1.84 (1)	2.6651 (6)	175 (1)
O3*W*—H3*WB*···O8^{ix}	0.85 (1)	2.03 (1)	2.8469 (6)	161 (1)
O4*W*—H4*WA*···O7	0.82 (1)	2.04 (1)	2.8552 (6)	173 (1)
O4*W*—H4*WB*···O8^{x}	0.81 (1)	2.00 (1)	2.7987 (7)	170 (1)
O5*W*—H5*WA*···O6	0.84 (1)	1.80 (1)	2.6359 (7)	172 (1)
O5*W*—H5*WB*···O5^{xi}	0.83 (1)	2.43 (1)	3.2184 (7)	159 (1)
O6*W*—H6*WA*···O8^{xi}	0.84 (1)	1.95 (1)	2.7557 (6)	159 (1)
O6*W*—H6*WB*···O2^{ii}	0.84 (1)	1.84 (1)	2.6508 (6)	160 (1)
O7*W*—H7*WA*···O2	0.86 (1)	1.77 (1)	2.6209 (6)	172 (1)
O7*W*—H7*WB*···O2^{ii}	0.85 (1)	2.12 (1)	2.9658 (6)	174 (1)
O8*W*—H8*WA*···O7^{ii}	0.83 (1)	1.95 (1)	2.7783 (7)	172 (1)
O8*W*—H8*WB*···O4^{v}	0.84 (1)	1.81 (1)	2.6220 (6)	164 (1)
O9*W*—H9*WA*···O5^{xii}	0.82 (1)	1.93 (1)	2.7531 (7)	174 (1)

O9*W*—H9*WB*···O3^{v}	0.84 (1)	1.90 (1)	2.7235 (6)	167 (1)
O10*W*—H10*A*···O7^{xii}	0.83 (1)	1.91 (1)	2.7345 (6)	175 (1)
O10*W*—H10*B*···O3^{vii}	0.85 (1)	1.85 (1)	2.6902 (6)	171 (1)
O11*W*—H11*A*···O6^{iii}	0.87 (1)	1.90 (1)	2.7666 (6)	173 (1)
O11*W*—H11*B*···O5^{ix}	0.85 (1)	2.00 (1)	2.8460 (7)	176 (1)
O12*W*—H12*A*···O6^{iii}	0.86 (1)	1.90 (1)	2.7438 (7)	168 (1)
O12*W*—H12*B*···O7^{xii}	0.85 (1)	1.97 (1)	2.8165 (6)	171 (1)

Symmetry codes: (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*+1, −*y*, −*z*; (v) *x*, *y*+1, *z*; (vii) −*x*+2, −*y*+1, −*z*+1; (viii) *x*, *y*−1, *z*; (ix) *x*+1, *y*, *z*; (x) −*x*, −*y*−1, −*z*; (xi) −*x*, −*y*, −*z*; (xii) *x*+1, *y*+1, *z*.

Trisodium orthophosphate heptahydrate (Na3PO4H2O7)

Crystal data

$Na_3(PO_4)(H_2O)_7$
M_r = 290.05
Orthorhombic, *Pca*2$_1$
a = 12.3169 (7) Å
b = 6.5324 (3) Å
c = 12.6602 (7) Å
V = 1018.63 (9) Å^3
Z = 4
F(000) = 600
D_x = 1.891 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9336 reflections
θ = 3.1–40.1°
μ = 0.44 mm^{-1}
T = 100 K
Fragment, colourless
0.28 × 0.19 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
ω– and *φ*–scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.695, T_{max} = 0.748
44325 measured reflections
6462 independent reflections
6108 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 40.5°, θ_{min} = 3.1°
h = −22→22
k = −11→11
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.046
S = 1.07
6462 reflections
192 parameters
15 restraints
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0225P)^2 + 0.0222P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Absolute structure: Flack *x* determined using 2767 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013).
Absolute structure parameter: 0.00 (3)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Na1	0.73222 (3)	0.61661 (6)	0.49574 (3)	0.00846 (6)
Na2	0.54849 (3)	0.70865 (6)	0.64923 (3)	0.00916 (6)
Na3	0.43297 (3)	1.27728 (6)	0.62867 (3)	0.00944 (6)
P1	0.75326 (2)	0.24872 (3)	0.32554 (2)	0.00477 (3)
O1	0.72833 (5)	0.47911 (9)	0.32845 (5)	0.00800 (9)
O2	0.66276 (5)	0.13564 (9)	0.38566 (5)	0.00924 (9)
O3	0.75902 (5)	0.16945 (10)	0.21082 (5)	0.00796 (9)
O4	0.86543 (5)	0.20695 (9)	0.37948 (5)	0.00788 (9)
O1W	0.57966 (5)	0.82117 (10)	0.47986 (5)	0.01029 (10)
H1WA	0.5198 (11)	0.815 (3)	0.4480 (14)	0.028 (4)*
H1WB	0.6126 (15)	0.921 (2)	0.4517 (17)	0.041 (6)*
O2W	0.88619 (5)	0.81072 (10)	0.45322 (5)	0.01096 (10)
H2WA	0.922 (2)	0.755 (3)	0.4035 (17)	0.057 (7)*
H2WB	0.8770 (15)	0.928 (2)	0.4281 (15)	0.035 (5)*
O3W	0.74117 (5)	0.75613 (10)	0.67442 (6)	0.00859 (10)
H3WA	0.7496 (13)	0.683 (3)	0.7294 (12)	0.019 (4)*
H3WB	0.7415 (12)	0.8842 (19)	0.6921 (16)	0.018 (4)*
O4W	0.60995 (5)	1.35459 (9)	0.56927 (5)	0.00912 (9)
H4WA	0.6198 (14)	1.287 (2)	0.5141 (11)	0.021 (4)*
H4WB	0.6484 (15)	1.283 (2)	0.6127 (14)	0.027 (5)*
O5W	0.37190 (5)	0.61919 (9)	0.57759 (5)	0.00872 (9)
H5WA	0.3356 (15)	0.691 (3)	0.6207 (13)	0.025 (4)*
H5WB	0.3699 (16)	0.688 (3)	0.5207 (12)	0.033 (5)*
O6W	0.49639 (5)	0.50744 (10)	0.79038 (7)	0.01433 (12)
H6WA	0.4324 (11)	0.504 (3)	0.8144 (15)	0.033 (5)*
H6WB	0.5315 (13)	0.419 (2)	0.8240 (15)	0.030 (5)*
O7W	0.48839 (5)	1.00429 (9)	0.73831 (5)	0.00970 (10)
H7WA	0.5377 (13)	1.056 (3)	0.7769 (14)	0.034 (5)*
H7WB	0.4388 (13)	0.965 (3)	0.7820 (13)	0.027 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.00824 (13)	0.00899 (14)	0.00816 (14)	−0.00015 (11)	0.00008 (11)	−0.00087 (12)
Na2	0.00823 (13)	0.01088 (14)	0.00835 (15)	−0.00081 (11)	0.00028 (11)	0.00097 (12)
Na3	0.00783 (13)	0.01056 (14)	0.00992 (15)	−0.00032 (11)	−0.00038 (11)	0.00150 (12)
P1	0.00497 (6)	0.00469 (6)	0.00464 (6)	−0.00022 (5)	0.00001 (6)	0.00026 (6)
O1	0.0102 (2)	0.00554 (19)	0.0083 (2)	0.00096 (15)	0.0004 (2)	0.00007 (19)
O2	0.0082 (2)	0.0103 (2)	0.0092 (2)	−0.00266 (18)	0.00143 (19)	0.0019 (2)
O3	0.0108 (2)	0.0076 (2)	0.0055 (2)	0.00040 (17)	−0.00007 (17)	−0.00092 (18)
O4	0.0058 (2)	0.0095 (2)	0.0083 (2)	0.00073 (17)	−0.00134 (17)	0.00040 (19)
O1W	0.0096 (2)	0.0104 (2)	0.0110 (3)	−0.00099 (18)	−0.0012 (2)	0.0037 (2)
O2W	0.0125 (2)	0.0097 (2)	0.0107 (3)	−0.0005 (2)	0.0010 (2)	0.0026 (2)
O3W	0.0102 (2)	0.0075 (2)	0.0081 (2)	0.00052 (17)	−0.00060 (18)	−0.00046 (18)
O4W	0.0087 (2)	0.0099 (2)	0.0088 (2)	0.00065 (17)	−0.00025 (19)	0.0004 (2)

O5W	0.0086 (2)	0.0095 (2)	0.0080 (2)	0.00113 (17)	0.0008 (2)	0.0004 (2)
O6W	0.0109 (2)	0.0158 (3)	0.0163 (3)	0.0056 (2)	0.0050 (2)	0.0084 (2)
O7W	0.0093 (2)	0.0105 (2)	0.0093 (3)	−0.0020 (2)	0.00029 (19)	0.00024 (18)

Geometric parameters (Å, º)

Na1—O1	2.3010 (8)	Na2—O4W^{i}	2.6357 (7)
Na1—O1W	2.3146 (7)	Na3—O4W	2.3605 (7)
Na1—O2W	2.3440 (7)	Na3—O7W	2.3606 (7)
Na1—O3W	2.4413 (8)	Na3—O2W^{iii}	2.3656 (8)
Na1—O4W^{i}	2.4626 (7)	Na3—O3W^{iii}	2.4421 (8)
Na1—O5W^{ii}	2.5311 (7)	Na3—O5W^{iv}	2.4439 (7)
Na2—O1W	2.2991 (7)	Na3—O6W^{iv}	2.6575 (10)
Na2—O6W	2.3093 (8)	P1—O1	1.5365 (6)
Na2—O7W	2.3558 (7)	P1—O2	1.5386 (6)
Na2—O3W	2.4146 (7)	P1—O3	1.5435 (7)
Na2—O5W	2.4279 (7)	P1—O4	1.5652 (6)
O1—Na1—O1W	97.38 (3)	Na2—O1W—H1WA	106.5 (13)
O1—Na1—O2W	90.95 (3)	Na1—O1W—H1WA	136.3 (14)
O1W—Na1—O2W	108.94 (3)	Na2—O1W—H1WB	135.9 (15)
O1—Na1—O3W	178.26 (3)	Na1—O1W—H1WB	95.4 (13)
O1W—Na1—O3W	84.36 (3)	H1WA—O1W—H1WB	104.9 (19)
O2W—Na1—O3W	88.53 (3)	Na1—O2W—Na3^{v}	81.37 (2)
O1—Na1—O4W^{i}	93.66 (2)	Na1—O2W—H2WA	110.7 (17)
O1W—Na1—O4W^{i}	86.42 (2)	Na3^{v}—O2W—H2WA	117.8 (19)
O2W—Na1—O4W^{i}	163.26 (3)	Na1—O2W—H2WB	118.3 (13)
O3W—Na1—O4W^{i}	86.38 (2)	Na3^{v}—O2W—H2WB	127.7 (14)
O1—Na1—O5W^{ii}	98.83 (2)	H2WA—O2W—H2WB	101 (2)
O1W—Na1—O5W^{ii}	159.85 (3)	Na2—O3W—Na1	77.60 (2)
O2W—Na1—O5W^{ii}	82.72 (2)	Na2—O3W—Na3^{v}	155.23 (4)
O3W—Na1—O5W^{ii}	79.46 (2)	Na1—O3W—Na3^{v}	77.91 (2)
O4W^{i}—Na1—O5W^{ii}	80.67 (2)	Na2—O3W—H3WA	99.0 (11)
O1W—Na2—O6W	161.83 (3)	Na1—O3W—H3WA	123.6 (14)
O1W—Na2—O7W	103.70 (3)	Na3^{v}—O3W—H3WA	91.4 (11)
O6W—Na2—O7W	90.51 (3)	Na2—O3W—H3WB	99.4 (10)
O1W—Na2—O3W	85.30 (3)	Na1—O3W—H3WB	126.9 (14)
O6W—Na2—O3W	104.12 (3)	Na3^{v}—O3W—H3WB	98.2 (10)
O7W—Na2—O3W	98.07 (3)	H3WA—O3W—H3WB	109.3 (18)
O1W—Na2—O5W	83.00 (2)	Na3—O4W—Na1^{iv}	146.50 (3)
O6W—Na2—O5W	84.44 (3)	Na3—O4W—Na2^{iv}	78.47 (2)
O7W—Na2—O5W	95.43 (2)	Na1^{iv}—O4W—Na2^{iv}	73.20 (2)
O3W—Na2—O5W	163.89 (3)	Na3—O4W—H4WA	106.6 (12)
O1W—Na2—O4W^{i}	82.79 (2)	Na1^{iv}—O4W—H4WA	88.0 (12)
O6W—Na2—O4W^{i}	82.97 (3)	Na2^{iv}—O4W—H4WA	145.9 (13)
O7W—Na2—O4W^{i}	173.46 (3)	Na3—O4W—H4WB	100.9 (14)
O3W—Na2—O4W^{i}	83.17 (2)	Na1^{iv}—O4W—H4WB	106.3 (13)
O5W—Na2—O4W^{i}	84.41 (2)	Na2^{iv}—O4W—H4WB	112.7 (13)

O4W—Na3—O7W	94.70 (3)	H4WA—O4W—H4WB	99.5 (17)
O4W—Na3—O2W^{iii}	88.73 (3)	Na2—O5W—Na3^{i}	81.11 (2)
O7W—Na3—O2W^{iii}	116.04 (3)	Na2—O5W—Na1^{vi}	155.28 (3)
O4W—Na3—O3W^{iii}	171.10 (3)	Na3^{i}—O5W—Na1^{vi}	76.19 (2)
O7W—Na3—O3W^{iii}	94.17 (3)	Na2—O5W—H5WA	95.7 (14)
O2W^{iii}—Na3—O3W^{iii}	88.02 (3)	Na3^{i}—O5W—H5WA	119.9 (13)
O4W—Na3—O5W^{iv}	90.25 (2)	Na1^{vi}—O5W—H5WA	104.0 (14)
O7W—Na3—O5W^{iv}	159.23 (3)	Na2—O5W—H5WB	102.5 (13)
O2W^{iii}—Na3—O5W^{iv}	84.18 (3)	Na3^{i}—O5W—H5WB	135.9 (15)
O3W^{iii}—Na3—O5W^{iv}	81.18 (2)	Na1^{vi}—O5W—H5WB	87.4 (14)
O4W—Na3—O6W^{iv}	81.54 (2)	H5WA—O5W—H5WB	103.7 (18)
O7W—Na3—O6W^{iv}	83.65 (3)	Na2—O6W—Na3^{i}	78.90 (3)
O2W^{iii}—Na3—O6W^{iv}	158.82 (3)	Na2—O6W—H6WA	123.6 (13)
O3W^{iii}—Na3—O6W^{iv}	98.76 (3)	Na3^{i}—O6W—H6WA	89.3 (13)
O5W^{iv}—Na3—O6W^{iv}	77.13 (2)	Na2—O6W—H6WB	129.9 (13)
O1—P1—O2	108.28 (3)	Na3^{i}—O6W—H6WB	98.9 (13)
O1—P1—O3	111.12 (4)	H6WA—O6W—H6WB	106.2 (18)
O2—P1—O3	109.74 (4)	Na2—O7W—Na3	115.38 (3)
O1—P1—O4	109.68 (3)	Na2—O7W—H7WA	112.1 (13)
O2—P1—O4	109.87 (4)	Na3—O7W—H7WA	104.2 (14)
O3—P1—O4	108.15 (4)	Na2—O7W—H7WB	106.6 (12)
P1—O1—Na1	113.60 (4)	Na3—O7W—H7WB	113.3 (12)
Na2—O1W—Na1	82.53 (2)	H7WA—O7W—H7WB	105 (2)

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) *x*+1/2, −*y*+1, *z*; (iii) *x*−1/2, −*y*+2, *z*; (iv) *x*, *y*+1, *z*; (v) *x*+1/2, −*y*+2, *z*; (vi) *x*−1/2, −*y*+1, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O4^{vi}	0.84 (1)	2.09 (1)	2.9344 (9)	176 (2)
O1*W*—H1*WB*···O2^{iv}	0.85 (1)	1.74 (1)	2.5865 (9)	172 (2)
O2*W*—H2*WA*···O6*W*^{vii}	0.85 (1)	2.38 (1)	3.2042 (11)	163 (2)
O2*W*—H2*WB*···O4^{iv}	0.84 (1)	1.93 (1)	2.7634 (9)	175 (2)
O3*W*—H3*WA*···O1^{viii}	0.85 (1)	1.85 (1)	2.6867 (9)	168 (2)
O3*W*—H3*WB*···O3^{ix}	0.87 (1)	1.88 (1)	2.7391 (9)	172 (2)
O4*W*—H4*WA*···O2^{iv}	0.84 (1)	1.97 (1)	2.8058 (9)	173 (2)
O4*W*—H4*WB*···O3^{ix}	0.86 (1)	1.84 (1)	2.6978 (9)	171 (2)
O5*W*—H5*WA*···O3^{x}	0.85 (1)	1.87 (1)	2.7114 (9)	173 (2)
O5*W*—H5*WB*···O4^{vi}	0.85 (1)	1.92 (1)	2.7544 (9)	169 (2)
O6*W*—H6*WA*···O1^{x}	0.85 (1)	1.99 (1)	2.8109 (9)	163 (2)
O6*W*—H6*WB*···O4^{viii}	0.84 (1)	2.01 (1)	2.8323 (9)	169 (2)
O7*W*—H7*WA*···O4^{ix}	0.85 (1)	2.02 (1)	2.8616 (9)	170 (2)
O7*W*—H7*WB*···O2^{x}	0.86 (1)	1.93 (1)	2.7894 (9)	175 (2)

Symmetry codes: (iv) *x*, *y*+1, *z*; (vi) *x*−1/2, −*y*+1, *z*; (vii) −*x*+3/2, *y*, *z*−1/2; (viii) −*x*+3/2, *y*, *z*+1/2; (ix) −*x*+3/2, *y*+1, *z*+1/2; (x) −*x*+1, −*y*+1, *z*+1/2.