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Sodium magnesium tris(dihydrogenphosphite) monohydrate, $NaMg(H_2PO_3)_3\cdot H_2O$

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The structure of $NaMg(H_2PO_3)_3\cdot H_2O$ belongs to the isotypic dihydrogenphosphite monohydrate series $NaM(H_2PO_3)_3\cdot H_2O$ (M = Mn, Co and Zn), with alternating NaO_6 [$d_{av}(Na-O)$ = 2.466 (2) Å] and MgO_6 [$d_{av}(Mg-O)$ = 2.086 (2) Å] octahedra, crosslinked by H_2PO_3 pseudo-pyramids [$d_{av}(P-OMg)$ = 1.530 (2) Å and $d_{av}(P-OH)$ = 1.575 (2) Å].

Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(Mg–O) = 0.002 Å
R factor = 0.027
wR factor = 0.066
Data-to-parameter ratio = 10.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

In the mixed phosphate system NaO–MO–H_3PO_3, where M is a bivalent 3d metal, only three compounds are known, *viz.* $NaM(H_2PO_3)_3\cdot H_2O$, with M = Mn (Chmelikova *et al.*, 1986), and M = Co (Kratochvíl *et al.*, 1982), and $NaZn(H_2PO_3)_3\cdot H_2O$ (Ouarsal *et al.*, 2002). In the present work, we describe the synthesis and crystal structure of the fourth member of the family, $NaMg(H_2PO_3)_3\cdot H_2O$, as part of our systematic investigation of this system.

The crystal structure of the title compound can be described as a three-dimensional network made of of [NaO_6] and [MgO_6] octahedra sharing edges by way of O3$\cdots$O8 and O6$\cdots$O7 pairs, as shown in Fig. 1. Cohesion of these polyhedra is further reinforced by the presence of O—P—O bridges of the [HPO_3H] units, through hydrogen bonds between the water oxygen and H atoms attached to O atoms of the phosphite groups. These bonds force the zigzag propagation of the chains along [010]. The chains are crosslinked by the phos-

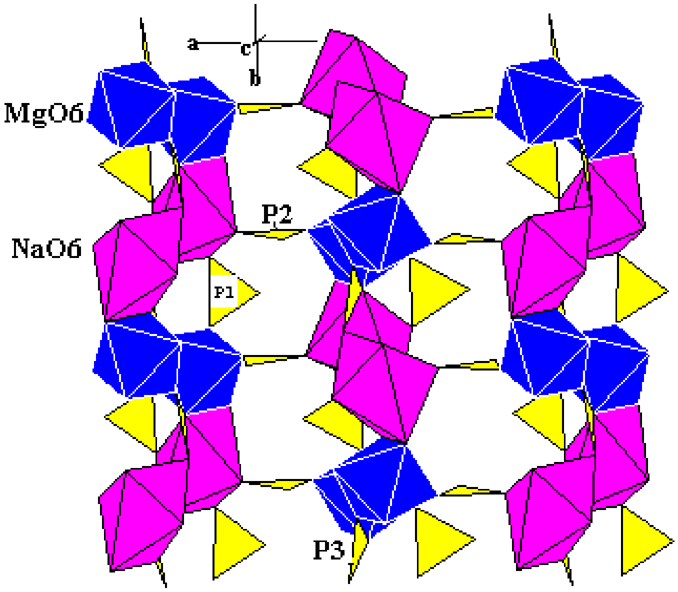

Figure 1
ATOMS (Dowty, 1999) projection of the crystal structure of $NaMg(H_2PO_3)_3\cdot H_2O$. Polyhedra: blue ($MgO_6$), pink ($NaO_6$) and yellow ($PO_3$) (H atoms are omitted for clarity).

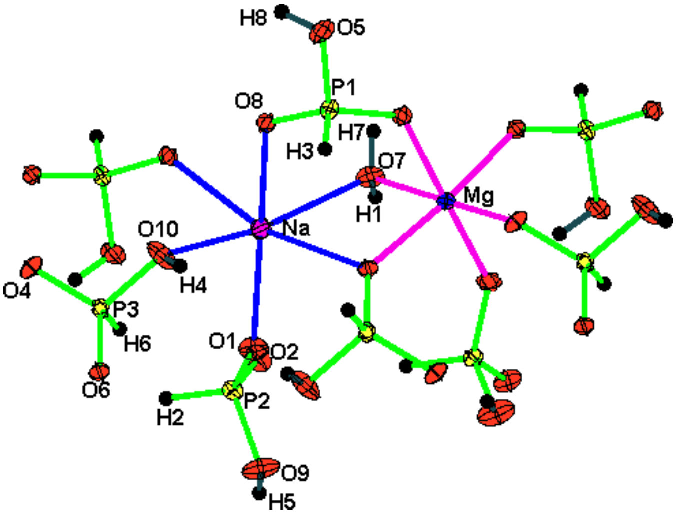

Figure 2
Coordination of Na and Zn in the crystal structure of NaMg(H_2PO_3)$_3$·H_2O. Atom colours are as for their polyhedra in Fig. 1; grey spheres (H). Displacement ellipsoids are drawn at the 50% probability level.

phite moieties: the P1- and P2-centered groups link adjacent chains in the *a* and *b* directions, respectively, while the P3-centered group acts in both directions. The P—OH···O and O*w*H···O (*w* is water) hydrogen bonds also stabilize the structure, as previously described by Chmelíková *et al.* (1986).

Phosphorous (P^{III}) atoms occupy three non-equivalent crystallographic positions. The surrounding tetrahedra consist of one hydroxyl, two non-hydroxyl O atoms and an H atom. Average P—O distances are 1.541, 1.525 and 1.525 Å, respectively. Average P—H and P—O(H) distances are 1.25 and 1.575 Å, respectively. They are similar to their equivalents in the homologous mixed phosphites, 1.500, 1.26 and 1.574 Å, respectively in NaMn(H_2PO_3)$_3$·H_2O and 1.501, 1.32 and 1.572 Å, respectively in NaZn(H_2PO_3)$_3$·H_2O.

Mg^{2+} is octahedrally coordinated by five O atoms of the phosphite anions and one oxygen (O7) of the water molecule. Average Mg—O is 2.086 Å, similar to that of 2.098 Å in Mg(H_2PO_3)$_2$·6H_2O (Corbridge, 1956). The Mg^{2+} ions are isolated in the structure, with Mg···Mg = 5.031 (2) Å, that is significantly shorter than the corresponding distance of 5.957 Å in Mg(H_2PO_3)$_2$·6H_2O.

Na^+ has a distorted octahedral coordination, with one Na—O distance longer than the others. The average Na–O, 2.466 Å, is similar to values found in isostructural phosphites: NaZn(H_2PO_3)$_3$·H_2O (2.451 Å), NaMn(H_2PO_3)$_3$·H_2O (2.442 Å). The bond-valence sum (Brown, 1996) for sodium, 1.15 (ideal value = 1.00), indicates that its valence is fully saturated. Fig. 2 shows the neighborhood of the Mg and Na atoms.

Experimental

The crystals were prepared by mixing the following two aqueous solutions: [NaOH (2.5 mmol) + H_3PO_3 (2.5 mmol)], [MgO (2.5 mmol) + H_3PO_3 (1.5 mmol)]. The mixture was stirred for 6 h and the resulting clear solution was left at room temperature for a few days. Large lozenge-shaped crystals were deposited; they were filtered off and washed with a solution of 80% ethanol.

Crystal data

$H_8MgNaO_{10}P_3$
$M_r = 308.3$
Orthorhombic, *Pbca*
$a = 14.806$ (1) Å
$b = 9.078$ (2) Å
$c = 14.811$ (2) Å
$V = 1990.8$ (5) Å^3
$Z = 8$
$D_x = 2.056$ Mg m^{-3}
Mo Kα radiation
Cell parameters from 45 reflections
$\theta = 10–15°$
$\mu = 0.74$ mm^{-1}
$T = 295$ K
Irregular polyhedron, colorless
0.3 × 0.2 × 0.1 mm

Data collection

Oxford Instruments KM-4 point detector diffractometer
$\theta/2\theta$ scans
Absorption correction: Gaussian (*JANA*2000; Petricek & Dusek, 2000)
$T_{\min} = 0.806$, $T_{\max} = 0.930$
10 838 measured reflections
2902 independent reflections
1760 reflections with $I > 3\sigma(I)$
$R_{\rm int} = 0.058$
$\theta_{\max} = 30.0°$
$h = -20 \rightarrow 20$
$k = 0 \rightarrow 12$
$l = -20 \rightarrow 20$
3 standard reflections every 100 reflections intensity decay: 1.3%

Refinement

Refinement on F^2
$R[F^2 > 3\sigma(F^2)] = 0.027$
$wR(F^2) = 0.066$
$S = 1.29$
1760 reflections
168 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(I) + 0.0016I^2]$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.38$ e Å^{-3}
$\Delta\rho_{\min} = -0.56$ e Å^{-3}

Table 1
Selected geometric parameters (Å).

P1—O3	1.5004 (16)	Mg1—O2$^{\rm i}$	2.1112 (18)
P1—O5	1.5864 (18)	Mg1—O3$^{\rm ii}$	2.0755 (17)
P1—O8	1.5003 (17)	Mg1—O4$^{\rm iii}$	2.0673 (18)
P1—H3	1.26 (3)	Mg1—O6	2.0594 (17)
P2—O1	1.4970 (17)	Mg1—O7	2.1498 (19)
P2—O2	1.5118 (17)	Mg1—O8	2.0529 (17)
P2—O9	1.568 (2)	Na1—O1	2.3303 (19)
P2—H2	1.25 (3)	Na1—O3$^{\rm iv}$	2.3481 (19)
P3—O4	1.5056 (17)	Na1—O6	2.4408 (19)
P3—O6	1.5005 (16)	Na1—O7	2.503 (2)
P3—O10	1.575 (2)	Na1—O8$^{\rm ii}$	2.3335 (18)
P3—H6	1.29 (3)	Na1—O10$^{\rm v}$	2.835 (2)

Symmetry codes: (i) $\frac{3}{2} - x, \frac{1}{2} + y, z$; (ii) $2 - x, y - \frac{1}{2}, \frac{1}{2} - z$; (iii) $2 - x, 1 - y, -z$; (iv) $x, y - 1, z$; (v) $2 - x, -y, -z$.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7···O10$^{\rm vi}$	0.87 (3)	2.17 (3)	3.020 (3)	168 (3)
O10—H4···O1	0.77 (4)	1.82 (4)	2.583 (3)	174 (5)
O7—H1···O5$^{\rm vii}$	0.74 (4)	2.05 (4)	2.777 (2)	165 (4)
O9—H5···O4$^{\rm vii}$	0.77 (4)	1.98 (4)	2.721 (3)	163 (4)
O5—H8···O2$^{\rm i}$	0.91 (3)	1.71 (3)	2.614 (2)	175 (3)

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

Data collection: *KM4B8* (Galdecki *et al.*, 1996); cell refinement: *KM4B8*; data reduction: *JANA*2000 (Petricek & Dusek, 2000); program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1997); program(s) used to refine structure: *JANA*2000; molecular graphics: *ATOMS* (Dowty, 1999); software used to prepare material for publication: *JANA*2000.

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