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Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
 Mean $\sigma(\text{Mg}-\text{O}) = 0.002\text{ \AA}$
 Disorder in main residue
 R factor = 0.033
 wR factor = 0.089
 Data-to-parameter ratio = 17.6

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

Potassium magnesium hydrogendiphosphate dihydrate

The title compound, $\text{KMg}(\text{HP}_2\text{O}_7)\cdot 2\text{H}_2\text{O}$, is isotypic with other members of the series $\text{KM}(\text{HP}_2\text{O}_7)\cdot 2\text{H}_2\text{O}$, where $M = \text{Mn}, \text{Co}$ and Zn . The structure consists of a three-dimensional framework of $[\text{MgHP}_2\text{O}_7]^-$ layers parallel to (100) linked by K^+ cations and hydrogen-bonding interactions. The metal ions and water O atoms lie on mirror planes, as does the bridging O atom of the eclipsed $(\text{HP}_2\text{O}_7)^{3-}$ anion. The acid H atom of the diphosphate anion is split into two half-occupied positions around a center of inversion.

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Comment

Acidic diphosphates are an important class of phosphates with many applications (Assaaoudi *et al.*, 2002; Essehli *et al.*, 2005, and references therein). The present paper deals with the synthesis and crystal structure of the Mg member of the series $\text{KM}(\text{HP}_2\text{O}_7)\cdot 2\text{H}_2\text{O}$, where M is a 3d divalent transition metal or Mg. $\text{KMg}(\text{HP}_2\text{O}_7)\cdot 2\text{H}_2\text{O}$ is isotypic with the known

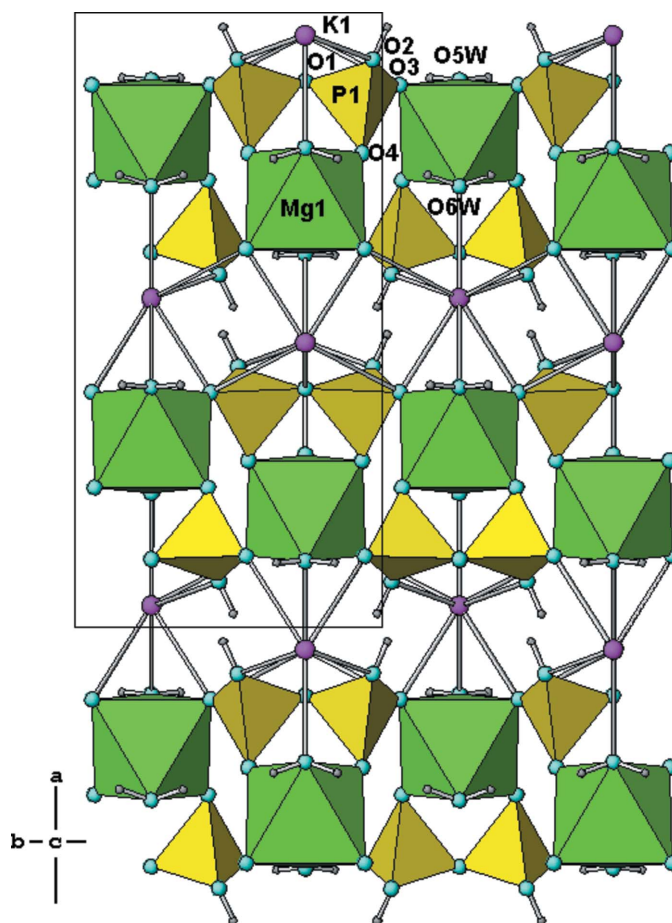


Figure 1
Projection of the $\text{KMg}(\text{HP}_2\text{O}_7)\cdot 2\text{H}_2\text{O}$ structure along the c axis.

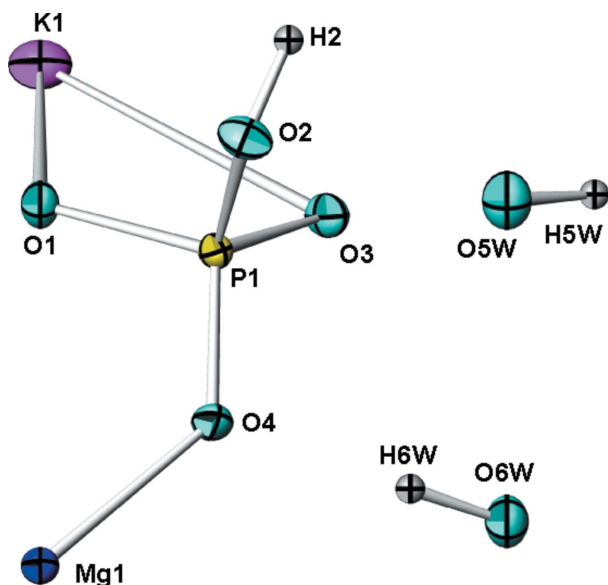


Figure 2
View of the asymmetric unit of $\text{KMg}(\text{HP}_2\text{O}_7)\cdot 2\text{H}_2\text{O}$, with displacement ellipsoids drawn at the 50% probability level. H atoms are given with arbitrary radius.

members of this series, where $M = \text{Mn}, \text{Zn}$ (Assaoudi *et al.*, 2002), and Co (Harcharras, Goubitz *et al.*, 2003).

The three-dimensional framework structure of $\text{KMg}(\text{HP}_2\text{O}_7)\cdot 2\text{H}_2\text{O}$ consists of acidic diphosphate metallate layers $[\text{MgHP}_2\text{O}_7]^-$ parallel to (100), linked by K^+ cations and hydrogen bonds (Fig. 1 and Table 2).

Mg^{2+} is octahedrally coordinated by six O atoms from three different $(\text{HP}_2\text{O}_7)^{3-}$ anions and two water molecules, the latter denoted as OW (Table 1). $[\text{MgO}_6]$ octahedra are isolated from each other in the structure. Two neighbouring $[\text{MgO}_6]$ octahedra are connected *via* O–P–O bridges from (HP_2O_7) groups. The average Mg–O distance of 2.09 (4) Å is comparable with the values observed for similar coordination polyhedra in other phosphates, as in $\text{K}_2\text{Mg}(\text{H}_2\text{P}_2\text{O}_7)_2\cdot 2\text{H}_2\text{O}$, where Mg–O = 2.071 Å (Harcharras, Capitelli *et al.*, 2003).

The bridging O atom (O1) of the hydrogendiphosphate anion is located on a mirror plane; thus, the asymmetric unit (Fig. 2) contains one unique P^{V} atom coordinated by four O atoms in a slightly distorted tetrahedral manner. The resulting $(\text{HP}_2\text{O}_7)^{3-}$ anion exhibits an eclipsed conformation, with a P–O1–P bridging angle of 129.80 (10)°. The bridging and average terminal P–O distances [1.6153 (8) and 1.52 (2) Å, respectively; Table 1] are of the usual magnitudes as reported for HP_2O_7 groups in the other isotypic hydrogen diphosphates: P–O_{ter} = 1.516 Å in both $\text{KMn}(\text{HP}_2\text{O}_7)\cdot 2\text{H}_2\text{O}$ and $\text{KZn}(\text{HP}_2\text{O}_7)\cdot 2\text{H}_2\text{O}$ (Assaoudi *et al.*, 2002), and P–O_{brid} = 1.613 and 1.616 Å in $\text{KMn}(\text{HP}_2\text{O}_7)\cdot 2\text{H}_2\text{O}$ and $\text{KZn}(\text{HP}_2\text{O}_7)\cdot 2\text{H}_2\text{O}$, respectively.

The average K–O distance of 3.0 (2) Å is in good agreement with K–O distances in the isotypic compounds $\text{KMn}(\text{HP}_2\text{O}_7)\cdot 2\text{H}_2\text{O}$ (2.965 Å) and $\text{KZn}(\text{HP}_2\text{O}_7)\cdot 2\text{H}_2\text{O}$ (2.951 Å).

Experimental

Crystals of the title compound were obtained by mixing equimolar quantities of $\text{K}_4\text{P}_2\text{O}_7$ and $\text{MgCl}_2\cdot 6\text{H}_2\text{O}$ in concentrated HCl (a few ml). The diphosphate was obtained by heating K_2HPO_4 at 873 K for 6 h. The solution was left at room temperature. After a week, well shaped large colourless crystals were deposited, which were washed with a solution of ethanol–water (80:20) and dried.

Crystal data

$\text{KMg}(\text{HP}_2\text{O}_7)(\text{H}_2\text{O})_2$
 $M_r = 274.39$
 Orthorhombic, $Pnma$
 $a = 15.5203$ (13) Å
 $b = 7.7786$ (6) Å
 $c = 6.4822$ (5) Å
 $V = 782.57$ (11) Å³
 $Z = 4$
 $D_x = 2.329$ Mg m⁻³

Mo $K\alpha$ radiation
 Cell parameters from 3218 reflections
 $\theta = 3.1$ – 31.8°
 $\mu = 1.19$ mm⁻¹
 $T = 293$ (2) K
 Prism, colourless
 0.14 × 0.12 × 0.10 mm

Data collection

Oxford Diffraction XCALIBUR-2
 CCD diffractometer
 ω scans
 Absorption correction: numerical
 (*CrysAlis RED*;
 Oxford Diffraction, 2004)
 $T_{\text{min}} = 0.754$, $T_{\text{max}} = 0.825$
 6826 measured reflections

1353 independent reflections
 1173 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$
 $\theta_{\text{max}} = 31.9^\circ$
 $h = -18 \rightarrow 22$
 $k = -11 \rightarrow 11$
 $l = -9 \rightarrow 9$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.089$
 $S = 1.05$
 1353 reflections
 77 parameters

H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0498P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.46$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.54$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

P1–O4	1.4986 (11)	K1–O5W ^{iv}	3.0074 (19)
P1–O3	1.5010 (11)	K1–O3 ^v	3.3490 (12)
P1–O2	1.5450 (11)	Mg1–O4 ^v	2.0447 (12)
P1–O1	1.6153 (8)	Mg1–O3 ^{vi}	2.0920 (12)
K1–O2 ⁱ	2.8225 (12)	Mg1–O5W ⁱⁱⁱ	2.1010 (19)
K1–O3 ⁱⁱ	2.8356 (12)	Mg1–O6W ^{vi}	2.1566 (18)
K1–O6W ⁱⁱⁱ	2.8652 (19)		
O4–P1–O3	115.61 (7)	O4–P1–O1	108.57 (7)
O4–P1–O2	110.32 (7)	O3–P1–O1	104.26 (7)
O3–P1–O2	111.76 (7)	O2–P1–O1	105.62 (8)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O6W–H6W ^{iv} ···O4	0.96 (2)	1.76 (2)	2.6864 (13)	161 (2)
O5W–H5W ^v ···O2 ^{vii}	0.99 (2)	1.85 (2)	2.8231 (13)	166 (2)
O2–H2 ^{vi} ···O2 ^v	0.91 (2)	1.57 (2)	2.455 (2)	161 (4)

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

H atoms were located in difference Fourier maps and refined with a common isotropic displacement parameter. The acid H atom (H2)

of the diphosphate anion was split into two half-occupied positions around a center of inversion.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2004); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2004); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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