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Key indicators

Single-crystal X-ray study
 $T = 292\text{ K}$
Mean $\sigma(\text{P}-\text{O}) = 0.004\text{ \AA}$
 R factor = 0.056
 wR factor = 0.093
Data-to-parameter ratio = 18.9

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

Dipotassium zinc bis(dihydrogendiphosphate) dihydrate, $\text{K}_2\text{Zn}(\text{H}_2\text{P}_2\text{O}_7)_2 \cdot 2\text{H}_2\text{O}$

The framework of $\text{K}_2\text{Zn}(\text{H}_2\text{P}_2\text{O}_7)_2 \cdot 2\text{H}_2\text{O}$ contains acid diphosphate–metallate layers linked by $\text{K} \cdots \text{O}$ interactions and weak hydrogen bonds. Zn^{2+} cations are coordinated octahedrally by O atoms from two bidentate $[\text{H}_2\text{P}_2\text{O}_7]^{2-}$ anions and two water molecules.

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Comment

To our knowledge, no mixed dihydrogendiphosphates of the form $(A,T)_x(\text{H}_2\text{P}_2\text{O}_7)_y \cdot z\text{H}_2\text{O}$ (A = alkaline earth and T = transition metal) have been reported. Some simple alkali metal dihydrogendiphosphates are known: $\text{Na}_2\text{H}_2\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$ (Collin & Willis, 1971), $\text{K}_2\text{H}_2\text{P}_2\text{O}_7$ (Larbot *et al.*, 1983), $\text{K}_2\text{H}_2\text{P}_2\text{O}_7 \cdot 0.5\text{H}_2\text{O}$ (Dumas *et al.*, 1973), $\text{K}_3\text{H}(\text{H}_2\text{P}_2\text{O}_7)_2$ (Dumas, 1978), $\text{K}_3\text{Na}(\text{H}_2\text{P}_2\text{O}_7)_2$ (Dumas *et al.*, 1980), $\text{Rb}_2\text{H}_2\text{P}_2\text{O}_7 \cdot 0.5\text{H}_2\text{O}$ (Averbuch-Pouchot & Durif, 1993*a*) and $\text{Cs}_2\text{H}_2\text{P}_2\text{O}_7$ (Averbuch-Pouchot & Durif, 1993*b*). Acidic metal diphosphates have been implicated in some enzyme-catalysed reaction processes (Haromy *et al.*, 1984) and are used as inhibitors in the formation and dissolution of apatite crystals *in vitro* (Mathew *et al.*, 1993). We recently reported the structures of two hydrogendiphosphates, $\text{KM}(\text{HP}_2\text{O}_7) \cdot 2\text{H}_2\text{O}$ ($M = \text{Mn}, \text{Zn}$) (Assaaoudi *et al.*, 2002). We report here the structure of the dihydrogendiphosphate $\text{K}_2\text{Zn}(\text{H}_2\text{P}_2\text{O}_7)_2 \cdot 2\text{H}_2\text{O}$.

The structure of $\text{K}_2\text{Zn}(\text{H}_2\text{P}_2\text{O}_7)_2 \cdot 2\text{H}_2\text{O}$ can be described in terms of layers parallel to (001) (Fig. 1). Each layer is built up of $[\text{KO}_8]$, $[\text{ZnO}_6]$ and $[\text{H}_2\text{P}_2\text{O}_7]$ polyhedra (Fig. 2), sharing

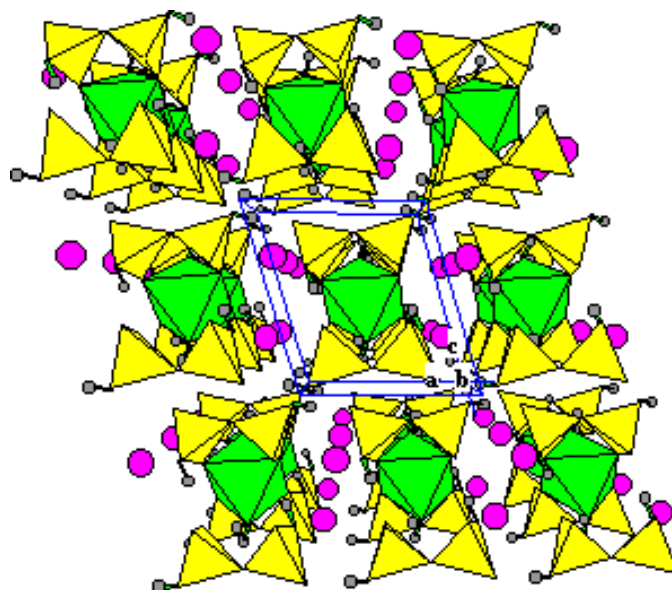


Figure 1
Projection along the b axis of $\text{K}_2\text{Zn}(\text{H}_2\text{P}_2\text{O}_7)_2 \cdot 2\text{H}_2\text{O}$. Polyhedra: yellow $[\text{H}_2\text{P}_2\text{O}_7]$, green $[\text{ZnO}_6]$; circles: large pink K, small grey H.

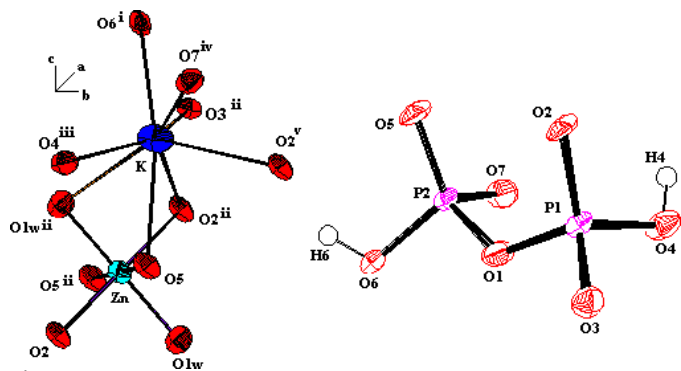


Figure 2
Coordination polyhedra of $[\text{KO}_8]$, $[\text{ZnO}_6]$ and $[\text{H}_2\text{P}_2\text{O}_7]$. Displacement ellipsoids are drawn at the 50% probability level.

corners and edges. The $[\text{ZnO}_6]$ polyhedra share four corners with two neighbouring $[\text{H}_2\text{P}_2\text{O}_7]$ anions to form the unit $[\text{Zn}(\text{H}_2\text{P}_2\text{O}_7)_2 \cdot 2\text{H}_2\text{O}]$, I. The $[\text{KO}_8]$ polyhedra share one edge to form the unit $[\text{K}_2\text{O}_{14}]$, II. Edge-sharing of units I and II results in a layer parallel to (001). Neighbouring layers are connected by $\text{K} \cdots \text{O}$ interactions and weak hydrogen bonds.

Each of the two unique phosphorus atoms is coordinated by four O atoms, one of which belongs to a hydroxyl group, in a slightly distorted tetrahedral geometry. The two tetrahedra share a corner (O1) to form the $[\text{H}_2\text{P}_2\text{O}_7]^{2-}$ anion in a roughly eclipsed conformation. The average P—O distance of 1.533 Å is similar to that found in $\text{K}_2\text{H}_2\text{P}_2\text{O}_7$ (1.537 Å) and $\text{K}_3\text{H}(\text{H}_2\text{P}_2\text{O}_7)_2$ (1.543 Å). The P—O—P angle of 128.85 (6)° is close to that in $\text{Ca}_2\text{P}_2\text{O}_7$ (130.0°; Calvo, 1968) and $\text{K}_4\text{P}_2\text{O}_7 \cdot 3\text{H}_2\text{O}$ (130.3°; Robertson & Calvo, 1967). The Zn^{2+} ions are coordinated in a nearly regular octahedral geometry by two bidentate $[\text{H}_2\text{P}_2\text{O}_7]^{2-}$ anions and two water molecules. The average Zn—O distance of 2.084 Å is close to that in $\beta\text{-Zn}_2\text{P}_2\text{O}_7$ (2.121 Å; Calvo, 1965). The $[\text{ZnO}_6]$ polyhedra are isolated, with the shortest Zn \cdots Zn distance being over 6 Å. The K atoms are eightfold coordinated, with K—O distances ranging from 2.757 (3) to 3.339 (4) Å. The average K—O distance of 2.959 Å is slightly longer than those found in $\text{K}_4\text{P}_2\text{O}_7 \cdot 3\text{H}_2\text{O}$ (2.812 Å; Dumas & Galigue, 1974) and $\text{K}_2\text{H}_2\text{P}_2\text{O}_7$ (2.908 Å; Larbot *et al.*, 1983).

Experimental

Stoichiometric amounts of ZnCl_2 were dissolved in a $\text{K}_4\text{P}_2\text{O}_7$ solution in distilled water. After it was stirred for 1 d and allowed to stand for two to three weeks, large prismatic colourless crystals were deposited. The crystals were filtered off and washed with a water–ethanol (20:80) solution.

Crystal data

$\text{K}_2\text{Zn}(\text{H}_2\text{P}_2\text{O}_7)_2 \cdot 2\text{H}_2\text{O}$
 $M_r = 531.51$
 Triclinic, $\overline{P}1$
 $a = 6.827$ (3) Å
 $b = 7.333$ (3) Å
 $c = 7.570$ (3) Å
 $\alpha = 80.753$ (8)°
 $\beta = 72.547$ (8)°
 $\gamma = 83.442$ (8)°
 $V = 356.0$ (2) Å³

$Z = 1$
 $D_x = 2.479$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 1307 reflections
 $\theta = 2.8\text{--}29.8^\circ$
 $\mu = 2.84$ mm⁻¹
 $T = 292$ (2) K
 Prism, colourless
 $0.33 \times 0.12 \times 0.04$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (XPREP; Sheldrick, 1997)
 $T_{\min} = 0.670$, $T_{\max} = 0.893$
 4313 measured reflections

2154 independent reflections
 1244 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.081$
 $\theta_{\text{max}} = 31.6^\circ$
 $h = -9 \rightarrow 9$
 $k = -10 \rightarrow 10$
 $l = -10 \rightarrow 10$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.056$
 $wR(F^2) = 0.093$
 $S = 0.86$
 2154 reflections
 114 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.001P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 1.28 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\text{min}} = -0.98 \text{ e } \text{Å}^{-3}$

Table 1

Selected geometric parameters (Å).

K1—O6 ⁱ	2.757 (3)	Zn1—O2	2.080 (3)
K1—O2 ⁱⁱ	2.775 (3)	Zn1—O1W ⁱⁱⁱ	2.116 (3)
K1—O4 ⁱⁱⁱ	2.874 (4)	Zn1—O1W	2.116 (3)
K1—O7 ^{iv}	2.899 (4)	P1—O3	1.485 (3)
K1—O1W ⁱⁱⁱ	2.941 (4)	P1—O2	1.490 (3)
K1—O5	2.949 (3)	P1—O4	1.556 (3)
K1—O2 ^v	3.139 (3)	P1—O1	1.589 (3)
K1—O3 ⁱⁱ	3.339 (4)	P2—O7	1.505 (3)
Zn1—O5 ⁱⁱ	2.057 (3)	P2—O5	1.499 (3)
Zn1—O5	2.057 (3)	P2—O6	1.536 (3)
Zn1—O2 ⁱⁱ	2.080 (3)	P2—O1	1.603 (3)

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

Table 2

Hydrogen-bonding geometry (Å, °).

$D\text{—}H \cdots A$	$D\text{—}H$	$H \cdots A$	$D \cdots A$	$D\text{—}H \cdots A$
O4—H4 \cdots O7 ⁱⁱⁱ	0.82	1.71	2.529 (5)	175
O6—H6 \cdots O3 ^v	0.82	1.70	2.503 (5)	165
O1W—H1W \cdots O3 ^{vi}	0.82	1.95	2.731 (5)	158
O1W—H2W \cdots O7 ^{vii}	0.78	2.00	2.775 (5)	171

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

The highest peak, at (0.3890, 0.5338, 0.4632), is 0.88 Å from Zn1, 1.51 Å from O2, 1.71 Å from O5 and 1.95 Å from O1W. H atoms were located in a difference Fourier map. The O—H distance was constrained to be the same for all H atoms; all other parameters, including U_{iso} , were refined freely.

Data collection: SMART (Bruker, 1999); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 (Farrugia, 1997) and ATOMS (Dowty, 1999); software used to prepare material for publication: SHELXL97.

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