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Rubidium zinc phosphate, $RbZn_2(PO_4)(HPO_4)$

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(P–O) = 0.004 Å
R factor = 0.054
wR factor = 0.063
Data-to-parameter ratio = 17.4

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

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Synthetic $RbZn_2(PO_4)(HPO_4)$ contains anionic layers of vertex-sharing ZnO_4 and $(H)PO_4$ tetrahedra [d_{av}(Zn—O) = 1.947 (4) Å and d_{av}(P—O) = 1.538 (4) Å]. The seven-coordinate Rb^+ cations [d_{av}(Rb—O) = 2.987 (4) Å] provide inter-layer charge compensation. $RbZn_2(PO_4)(HPO_4)$ is isostructural with its potassium and ammonium congeners.

Comment

The title compound (Figs. 1 and 2) is isostructural with $KZn_2(PO_4)(HPO_4)$ (Averbuch-Pouchot, 1979) and $NH_4Zn_2(PO_4)(HPO_4)$ (Bircsak & Harrison, 1998). The ZnO_4 and $(H)PO_4$ moieties assemble into corrugated anionic layers normal to [001]. Bicoordinate Zn—O—P and tricoordinate Zn—O—(Zn,P) O atoms occur in these layers (Bircsak & Harrison, 1998). The $[Zn_2(PO_4(HPO_4)]^-$ sheets are connected by seven-coordinate inter-layer Rb^+ species and O7—H1···O8 hydrogen bonds.

Experimental

The reaction was carried out in a polypropylene bottle: 1.365 g of $Zn(NO_3)_2$ was dissolved in 10 ml 1 M H_3PO_4 solution resulting in a clear solution. Then, 4.217 g of 50% RbOH solution was added, resulting in a white gel. The bottle was capped, shaken well, and placed in a 343 K oven for 24 h. The crystalline product was recovered by vacuum filtration and washing with acetone.

Crystal data

$RbZn_2(PO_4)(HPO_4)$
M_r = 407.17
Triclinic, $P\overline{1}$
a = 5.2605 (4) Å
b = 8.9046 (6) Å
c = 9.7244 (7) Å
α = 75.685 (1)°
β = 77.487 (2)°
γ = 73.489 (1)°
V = 417.89 (6) Å^3
Z = 2
D_x = 3.236 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2016 reflections
θ = 2.2–30.0°
μ = 11.92 mm^{-1}
T = 298 K
Rod, colourless
0.30 × 0.05 × 0.04 mm

Data collection

Bruker SMART1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.318, T_{max} = 0.746
3620 measured reflections
2385 independent reflections
2084 reflections with $I > \sigma(I)$
R_{int} = 0.033
θ_{max} = 30.0°
$h = -5 \rightarrow 7$
$k = -12 \rightarrow 12$
$l = -13 \rightarrow 12$

Refinement

Refinement on F
R = 0.054
wR = 0.063
S = 1.07
2084 reflections
120 parameters
Only H-atom U's refined
Weighting: Chebychev polynomial with 3 parameters (Carruthers & Watkin, 1979) 1.08 0.848 0.686
$(\Delta/\sigma)_{max}$ = 0.0004
$\Delta\rho_{max}$ = 1.18 e Å^{-3}
$\Delta\rho_{min}$ = −1.86 e Å^{-3}
Extinction correction: Larson (1967)
Extinction coefficient: 8.6 (31)

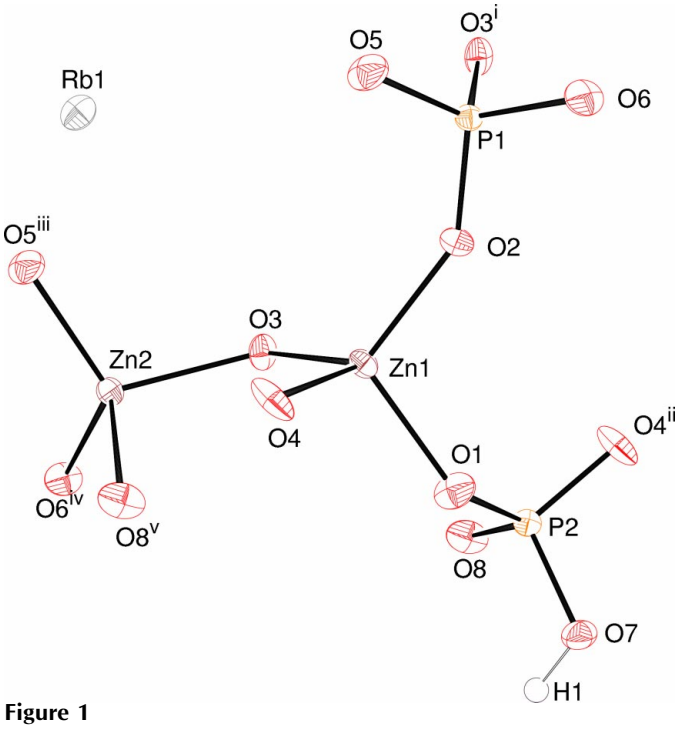

Figure 1
Fragment of $RbZn_2(PO_4)(HPO_4)$ (50% displacement ellipsoids, symmetry codes as in Table 1).

Table 1
Selected geometric parameters (Å, °).

Rb1—O1	2.936 (4)	Zn2—O5^{iv}	1.914 (4)
Rb1—O2^{i}	2.956 (4)	Zn2—O6^{v}	1.911 (4)
Rb1—O4^{ii}	2.825 (4)	Zn2—O8^{iii}	1.989 (4)
Rb1—O5^{ii}	3.096 (4)	P1—O2	1.527 (4)
Rb1—O6^{i}	2.922 (4)	P1—O3^{vi}	1.574 (4)
Rb1—O7^{iii}	2.902 (4)	P1—O5	1.511 (4)
Rb1—O7	3.275 (4)	P1—O6	1.532 (4)
Zn1—O1	1.933 (4)	P2—O1	1.519 (4)
Zn1—O2	1.896 (4)	P2—O4^{vii}	1.522 (4)
Zn1—O3	1.965 (3)	P2—O7	1.583 (4)
Zn1—O4	1.948 (4)	P2—O8	1.536 (4)
Zn2—O3	2.017 (4)		
Zn1—O1—P2	132.1 (3)	Zn1—O4—P2^{iii}	128.6 (2)
Zn1—O2—P1	148.1 (3)	Zn2^{iv}—O5—P1	143.0 (3)
Zn1—O3—Zn2	117.15 (18)	Zn2^{viii}—O6—P1	138.1 (3)
Zn1—O3—P1^{vi}	126.0 (2)	Zn2^{vii}—O8—P2	126.7 (2)
Zn2—O3—P1^{vi}	113.76 (19)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H1···O8^{i}	0.934	1.694	2.605 (6)	164

Symmetry code: (i) $2-x, -y, 2-z$.

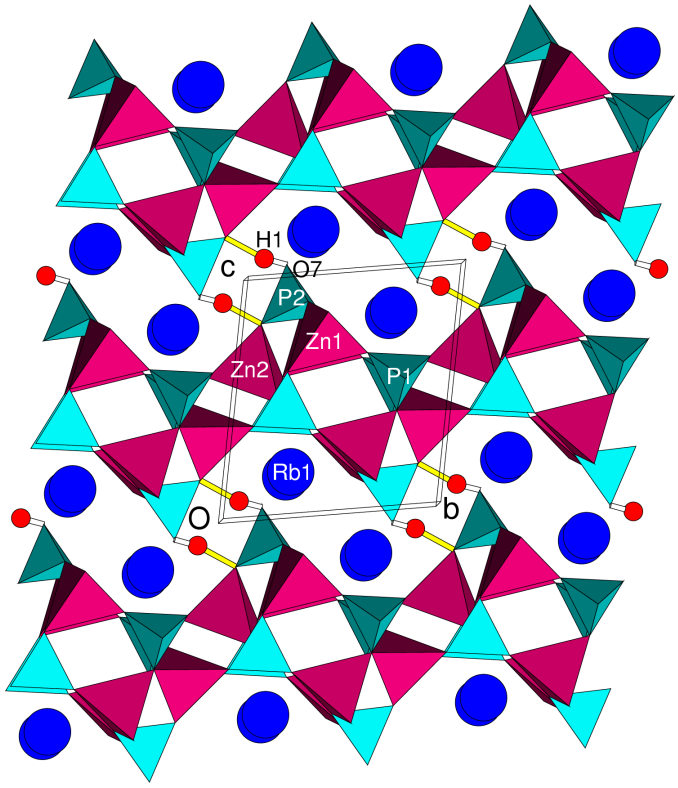

Figure 2
Polyhedral plot of $RbZn_2(PO_4)(HPO_4)$ viewed down [100]. Colour codes: ZnO_4 groups maroon, PO_4 groups light blue, Rb atoms dark blue, H atoms red, O—H bonds white and H···O interactions yellow.

The highest difference peak is 0.86 Å fron Zn2 and the deepest difference hole is 0.82 Å fron Zn1.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SMART*; data reduction: *SMART*; program(s) used to refine structure: *CRYSTALS* (Watkin *et al.*, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997).; software used to prepare material for publication: *CRYSTALS*.

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