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The triclinic form of dipotassium cobalt(II) bis(dihydrogendiphosphate) dihydrate

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Key indicators: single-crystal X-ray study; T = 292 K; mean σ(Co–O) = 0.003 Å; R factor = 0.038; wR factor = 0.090; data-to-parameter ratio = 12.6.

In the title compound, $K_2Co(H_2P_2O_7)_2\cdot 2H_2O$, the octahedrally coordinated Co^{2+} ion lies on an inversion centre. Two bidentate dihydrogendiphosphate anions form the equatorial plane of the $[CoO_6]$ octahedron which is completed by two water molecules in axial positions. This results in isolated $\{Co(H_2O)_2[H_2P_2O_7]_2\}^{4-}$ entities linked into a three-dimensional network through K—O bonds and O—H···O hydrogen-bonding interactions involving the dihydrogendiphosphate anions and water molecules. The dihydrogendiphosphate anion, $(H_2P_2O_7)^{2-}$, is bent and shows an almost eclipsed conformation.

Related literature

The triclinic title compound is isotypic with $K_2Ni(H_2P_2O_7)_2\cdot 2H_2O$ (Tahiri *et al.*, 2004) and $K_2Zn(H_2P_2O_7)_2\cdot 2H_2O$ (Tahiri *et al.*, 2003). For orthorhombic forms of crystals of this formula type, see: Tahiri *et al.* (2002); Essehli *et al.* (2005).

Experimental

Crystal data

$K_2Co(H_2P_2O_7)_2\cdot 2H_2O$
M_r = 525.1
Triclinic, $P\overline{1}$
a = 6.8737 (14) Å
b = 7.3565 (11) Å
c = 7.6141 (14) Å
α = 80.740 (14)°
β = 72.397 (17)°
γ = 83.484 (14)°
V = 361.35 (12) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 2.29 mm^{-1}
T = 292 K
0.16 × 0.11 × 0.03 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire 2 CCD detector
Absorption correction: analytical based on the crystal shape (*CrysAlis RED*; Oxford Diffraction, 2004)
T_{min} = 0.648, T_{max} = 0.838
4546 measured reflections
1489 independent reflections
1013 reflections with $I > 3\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.090
S = 1.17
1489 reflections
118 parameters
Only H-atom coordinates refined
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

K1—O2^{i}	2.785 (3)	P1—O1	1.602 (3)
K1—O4^{ii}	2.884 (3)	P1—O2	1.495 (3)
K1—O5	2.979 (3)	P1—O3	1.496 (3)
K1—O6^{iii}	2.771 (4)	P1—O4	1.556 (3)
K1—O7^{iv}	2.919 (3)	P2—O1	1.602 (3)
K1—O8^{i}	2.972 (4)	P2—O5	1.493 (3)
Co1—O2	2.101 (3)	P2—O6	1.546 (3)
Co1—O5	2.085 (3)	P2—O7	1.499 (3)
Co1—O8	2.094 (3)		
P1—O1—P2	130.90 (19)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H1···O7^{ii}	0.81 (5)	1.75 (5)	2.545 (5)	169 (5)
O6—H2···O3^{v}	0.72 (6)	1.82 (6)	2.522 (5)	168 (5)
O8—H3···O3^{vi}	0.71 (5)	2.03 (5)	2.745 (4)	178 (6)
O8—H4···O7^{vii}	0.79 (5)	2.01 (6)	2.798 (5)	175 (5)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2004); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2004); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *JANA2006* (Petříček *et al.*, 2006); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *JANA2006*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2482).

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The triclinic form of dipotassium cobalt(II) bis(dihydrogendiphosphate) dihydrate

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S1. Comment

The triclinic form of $K_2Co(H_2P_2O_7)_2{\cdot}2H_2O$ is isotypic with $K_2Ni(H_2P_2O_7)_2{\cdot}2H_2O$ (Tahiri *et al.*, 2004) and $K_2Zn(H_2P_2O_7)_2{\cdot}2H_2O$ (Tahiri *et al.*, 2003). All these $K_2M(H_2P_2O_7)_2{\cdot}2H_2O$ dihydrogendiphosphates crystallise also in an orthorhombic form, see: Tahiri *et al.* (2002) for *M* = Co; Essehli *et al.* (2005) for *M* = Ni and Zn.

The crystal structure of the title compound can be described in terms of centrosymmetric $\{Co(H_2O)_2[H_2P_2O_7]_2\}^{4-}$ units (Fig. 1) that are linked through K—O bonds and an intricate network of O—H···O hydrogen bonds into a three-dimensional network (Fig. 2). The slightly distorted coordination octahedron around Co^{2+} is composed of four O atoms from two bidendate $[H_2P_2O_7]^{2-}$ groups in equatorial positions and two O atoms from water molecules in axial positions. The average Co—O bond length of 2.093 (8) Å is in the same range as 2.047 Å for the orthorhombic form (Tahiri *et al.*, 2002). The dihydrogendiphosphate anion is bent and shows an almost eclipsed conformation, with an bridging angle P1—O1—P2 of 130.90 (19) °. P—O bond lengths and O—P—O angles values are of similar values as in known dihydrogendiphosphates. The K^+ cation is coordinated by six O atoms in form of a very distorted octahedron, with K—O distances ranging from 2.771 (4) to 2.979 (3) Å. Such values are likewise found in isotypic or isoformular dihydrogendiphosphates.

S2. Experimental

To prepare the present crystals we used the same procedure as described in detail in (Tahiri *et al.*, 2002). Solutions of $CoCl_2{\cdot}4H_2O$ (10 ml, 10 mmol) and $K_4P_2O_7$ (10 ml, 20 mmol) were mixed in a beaker. The mixture was stirred for six hours and then allowed to stand for two weeks at room temperature. At the end of this period, large prismatic pink crystals have deposited, which were filtered-off and washed with a water-ethanol solution (20:80).

S3. Refinement

All hydrogen atoms were found in difference Fourier maps and their coordinates were refined independently. The isotropic atomic displacement parameters of hydrogen atoms were treated with $1.2\times U_{eq}$ of the respective parent O atom.

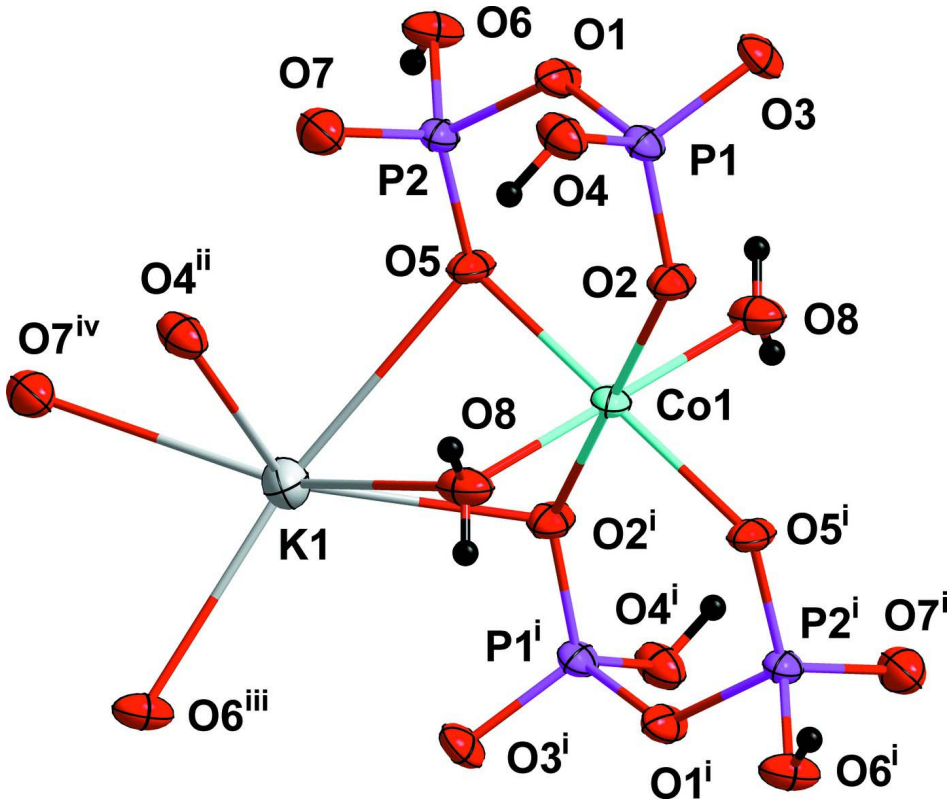

Figure 1

The main coordination polyhedra in the title compound, shown as an ellipsoid plot with anisotropic displacement parameters drawn at the 50% probability level. [Symmetry codes: (i) 1 - *x*, 1 - *y*, 1 - *z*; (ii) 1 - *x*, -*y*, 1 - *z*; (iii) *x*, *y*, 1 + *z*; (iv) 2 - *x*, -*y*, 1 - *z*].

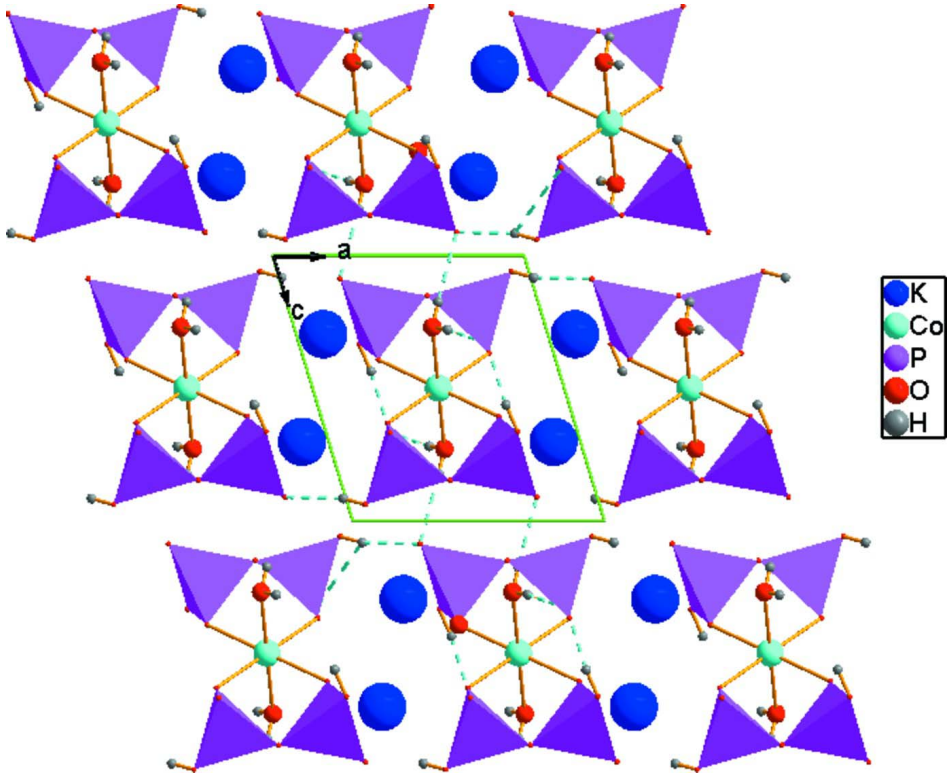

Figure 2

Projection of the structure along the *b*-axis. H-bonds are displayed as dashed lines.

dipotassium cobalt(II) bis(dihydrogendiphosphate) dihydrate

Crystal data

$K_2Co(H_2P_2O_7)_2{\cdot}2H_2O$
$M_r = 525.1$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.8737\ (14)$ Å
$b = 7.3565\ (11)$ Å
$c = 7.6141\ (14)$ Å
$\alpha = 80.740\ (14)°$
$\beta = 72.397\ (17)°$
$\gamma = 83.484\ (14)°$
$V = 361.35\ (12)$ Å^3
$Z = 1$
$F(000) = 261$
$D_x = 2.412$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 4546 reflections
$\theta = 3.1–26.6°$
$\mu = 2.29$ mm^{-1}
$T = 292$ K
Prism, pink
0.16 × 0.11 × 0.03 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire 2 CCD detector
Radiation source: Mo X-ray tube
Graphite monochromator
Detector resolution: 8.3438 pixels mm^{-1}
Rotation method data acquisition using ω scans
Absorption correction: analytical based on the crystal shape (*CrysAlis RED*; Oxford Diffraction, 2004)
$T_{min} = 0.648$, $T_{max} = 0.838$
4546 measured reflections
1489 independent reflections
1013 reflections with $I > 3\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 26.6°$, $\theta_{min} = 3.1°$
$h = -8\rightarrow8$
$k = -9\rightarrow9$
$l = -9\rightarrow9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.090$
$S = 1.17$
1489 reflections
118 parameters
0 restraints
4 constraints
Only H-atom coordinates refined
Weighting scheme based on measured s.u.'s $w = 1/[\sigma^2(I) + 0.0016I^2]$
$(\Delta/\sigma)_{max} = 0.044$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.45$ e Å^{-3}

Special details

Refinement. The hydrogen atoms were localized from the difference Fourier map. Their coordinates were refined independently. The isotropic temperature parameters of hydrogen atoms were calculated as $1.2*U_{eq}$ of the parent atom.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
K1	0.89288 (17)	0.26574 (14)	0.70307 (15)	0.0365 (4)
Co1	0.5	0.5	0.5	0.0172 (3)
P1	0.32488 (16)	0.27153 (14)	0.24623 (14)	0.0181 (4)
P2	0.75153 (16)	0.18965 (14)	0.24070 (14)	0.0177 (4)
O1	0.5649 (4)	0.2309 (4)	0.1518 (4)	0.0242 (11)
O2	0.2951 (4)	0.3930 (4)	0.3932 (4)	0.0213 (10)
O3	0.2401 (4)	0.3486 (4)	0.0882 (4)	0.0241 (10)
O4	0.2372 (5)	0.0812 (4)	0.3353 (4)	0.0263 (11)
H1	0.252 (7)	0.045 (6)	0.437 (6)	0.0316*
O5	0.7435 (4)	0.3267 (4)	0.3681 (4)	0.0231 (10)
O6	0.9309 (4)	0.2143 (4)	0.0601 (4)	0.0258 (11)
H2	1.011 (7)	0.252 (7)	0.083 (7)	0.0309*
O7	0.7467 (5)	−0.0072 (4)	0.3310 (4)	0.0283 (11)
O8	0.5496 (5)	0.7064 (4)	0.2702 (4)	0.0274 (12)
H3	0.602 (8)	0.692 (7)	0.176 (7)	0.0329*
H4	0.606 (7)	0.790 (7)	0.280 (7)	0.0329*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K1	0.0433 (6)	0.0353 (6)	0.0362 (6)	0.0096 (5)	−0.0215 (5)	−0.0093 (5)
Co1	0.0201 (4)	0.0177 (4)	0.0175 (4)	0.0005 (3)	−0.0093 (3)	−0.0069 (3)
P1	0.0183 (5)	0.0215 (6)	0.0184 (5)	−0.0008 (4)	−0.0095 (4)	−0.0062 (4)
P2	0.0193 (5)	0.0204 (6)	0.0166 (5)	0.0009 (4)	−0.0084 (4)	−0.0068 (4)
O1	0.0183 (15)	0.0363 (18)	0.0229 (15)	0.0048 (12)	−0.0110 (12)	−0.0128 (13)
O2	0.0212 (15)	0.0236 (15)	0.0238 (15)	−0.0009 (12)	−0.0095 (12)	−0.0110 (12)
O3	0.0222 (16)	0.0337 (17)	0.0198 (15)	−0.0011 (13)	−0.0130 (13)	−0.0008 (13)
O4	0.0359 (18)	0.0235 (16)	0.0238 (17)	−0.0081 (13)	−0.0143 (15)	−0.0005 (13)
O5	0.0225 (16)	0.0294 (16)	0.0225 (15)	0.0037 (13)	−0.0099 (13)	−0.0156 (13)
O6	0.0215 (17)	0.0403 (19)	0.0180 (15)	−0.0081 (14)	−0.0039 (13)	−0.0105 (14)
O7	0.0388 (18)	0.0224 (16)	0.0269 (17)	−0.0040 (14)	−0.0137 (14)	−0.0024 (13)
O8	0.039 (2)	0.0253 (18)	0.0188 (16)	−0.0079 (15)	−0.0065 (15)	−0.0063 (14)

Geometric parameters (Å, º)

K1—O2^{i}	2.785 (3)	Co1—O8^{i}	2.094 (3)
K1—O4^{ii}	2.884 (3)	P1—O1	1.602 (3)
K1—O5	2.979 (3)	P1—O2	1.495 (3)
K1—O6^{iii}	2.771 (4)	P1—O3	1.496 (3)
K1—O7^{iv}	2.919 (3)	P1—O4	1.556 (3)
K1—O8^{i}	2.972 (4)	P2—O1	1.602 (3)
Co1—O2	2.101 (3)	P2—O5	1.493 (3)
Co1—O2^{i}	2.101 (3)	P2—O6	1.546 (3)
Co1—O5	2.085 (3)	P2—O7	1.499 (3)
Co1—O5^{i}	2.085 (3)	O4—H1	0.81 (5)
Co1—O8	2.094 (3)	O6—H2	0.72 (6)
O2^{i}—K1—O4^{ii}	123.43 (10)	O5^{i}—Co1—O5	180
O2^{i}—K1—O5	60.33 (9)	O5^{i}—Co1—O8	86.81 (11)
O2^{i}—K1—O6^{iii}	113.92 (10)	O5^{i}—Co1—O8^{i}	93.19 (11)
O2^{i}—K1—O7^{iv}	151.28 (8)	O8^{i}—Co1—O8	180
O2^{i}—K1—O8^{i}	60.69 (9)	O1—P1—O2	109.27 (18)
O4^{ii}—K1—O5	72.55 (9)	O1—P1—O3	105.02 (15)
O4^{ii}—K1—O6^{iii}	104.16 (10)	O1—P1—O4	106.45 (15)
O4^{ii}—K1—O7^{iv}	74.58 (9)	O2—P1—O3	116.17 (17)
O4^{ii}—K1—O8^{i}	68.68 (9)	O2—P1—O4	110.05 (16)
O5—K1—O6^{iii}	166.01 (9)	O3—P1—O4	109.36 (19)
O5—K1—O7^{iv}	113.42 (9)	O1—P2—O5	110.97 (16)
O5—K1—O8^{i}	57.71 (8)	O1—P2—O6	98.96 (17)
O6^{iii}—K1—O7^{iv}	77.87 (9)	O1—P2—O7	107.47 (18)
O6^{iii}—K1—O8^{i}	108.32 (9)	O5—P2—O6	112.65 (18)
O7^{iv}—K1—O8^{i}	143.17 (10)	O5—P2—O7	114.33 (17)
O2—Co1—O2^{i}	180	O6—P2—O7	111.27 (17)
O2—Co1—O5	92.27 (11)	P1—O1—P2	130.90 (19)
O2—Co1—O5^{i}	87.73 (11)	K1^{i}—O2—Co1	95.37 (10)
O2—Co1—O8	87.94 (13)	K1^{i}—O2—P1	110.42 (15)
O2—Co1—O8^{i}	92.06 (13)	Co1—O2—P1	132.80 (16)
O2^{i}—Co1—O2	180	K1^{ii}—O4—P1	150.05 (19)
O2^{i}—Co1—O5	87.73 (11)	P1—O4—H1	114 (4)
O2^{i}—Co1—O5^{i}	92.27 (11)	K1—O5—Co1	90.21 (10)
O2^{i}—Co1—O8	92.06 (13)	K1—O5—P2	127.17 (15)
O2^{i}—Co1—O8^{i}	87.94 (13)	Co1—O5—P2	130.12 (19)
O5—Co1—O5^{i}	180	K1^{v}—O6—P2	125.12 (18)
O5—Co1—O8	93.19 (11)	P2—O6—H2	107 (4)
O5—Co1—O8^{i}	86.81 (11)	H3—O8—H4	101 (5)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H1···O7^{ii}	0.81 (5)	1.75 (5)	2.545 (5)	169 (5)

O6—H2···O3^{vi}	0.72 (6)	1.82 (6)	2.522 (5)	168 (5)
O8—H3···O3^{vii}	0.71 (5)	2.03 (5)	2.745 (4)	178 (6)
O8—H4···O7^{viii}	0.79 (5)	2.01 (6)	2.798 (5)	175 (5)

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