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Cobalt potassium dihydrogendiphosphate dihydrate, $CoK_2(H_2P_2O_7)_2\cdot 2H_2O$

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(P–O) = 0.001 Å
R factor = 0.024
wR factor = 0.061
Data-to-parameter ratio = 19.1

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

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The crystal structure of the title compound, $CoK_2(H_2P_2O_7)_2\cdot 2H_2O$, is, to our knowledge, the first example of a mixed-metal dihydrogendiphosphate, containing an alkali earth metal and a divalent transition metal. The metal ions and the two water O atoms are located on a crystallographic mirror plane.

Comment

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Experimental

Crystals were prepared by dissolving an equimolar amount of $CoCl_2\cdot 6H_2O$ in a solution made of $K_4P_2O_7$ in distilled water. The mixture was stirred for 1 d and the resulting light-pink solution was allowed to stand at room temperature. After two to three weeks, pink crystals deposited; they were filtered off and washed with an aqueous solution.

Crystal data

$[CoK_2(H_2P_2O_7)_2]\cdot 2H_2O$
M_r = 525.07
Orthorhombic, *Pnma*
a = 9.7044 (5) Å
b = 11.0023 (6) Å
c = 13.3937 (8) Å
V = 1430.05 (14) Å^3
Z = 4
D_x = 2.439 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 28672 reflections
θ = 3.6–31.3°
μ = 2.32 mm^{-1}
T = 173 (2) K
Block, light pink
0.22 × 0.18 × 0.09 mm

Data collection

Stoe IPDS II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 1990; Blessing, 1995)
T_{min} = 0.630, T_{max} = 0.819
24419 measured reflections
2441 independent reflections
2173 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 31.4°
$h = -11 \rightarrow 14$
$k = -16 \rightarrow 16$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.061
S = 1.03
2441 reflections
128 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0413P)^2 + 0.057P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.70 e Å^{-3}

Table 1
Selected geometric parameters (Å).

Co1—O6	2.0883 (10)	K1—O9^{iii}	2.9636 (16)
Co1—O2	2.0926 (10)	K2—O5	2.7007 (10)
Co1—O9	2.1018 (14)	K2—O2^{iv}	2.8149 (10)
Co1—O8	2.1537 (15)	K2—O8^{iv}	2.9951 (17)
K1—O3^{i}	2.6975 (11)	K2—O6^{v}	3.0239 (12)
K1—O1	2.6982 (11)	K2—O8^{vi}	3.2827 (17)
K1—O6^{ii}	2.9621 (10)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O7^{i}	0.78 (3)	1.76 (3)	2.5272 (15)	170 (4)
O5—H5···O1^{ii}	0.76 (3)	1.74 (3)	2.4996 (15)	176 (3)
O8—H8···O2^{iii}	0.81 (3)	2.07 (3)	2.8255 (17)	156 (3)
O9—H9···O7^{iv}	0.85 (3)	1.92 (3)	2.7669 (14)	175 (3)

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

All H atoms could be located in a difference Fourier synthesis and were refined isotropically.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL*97.

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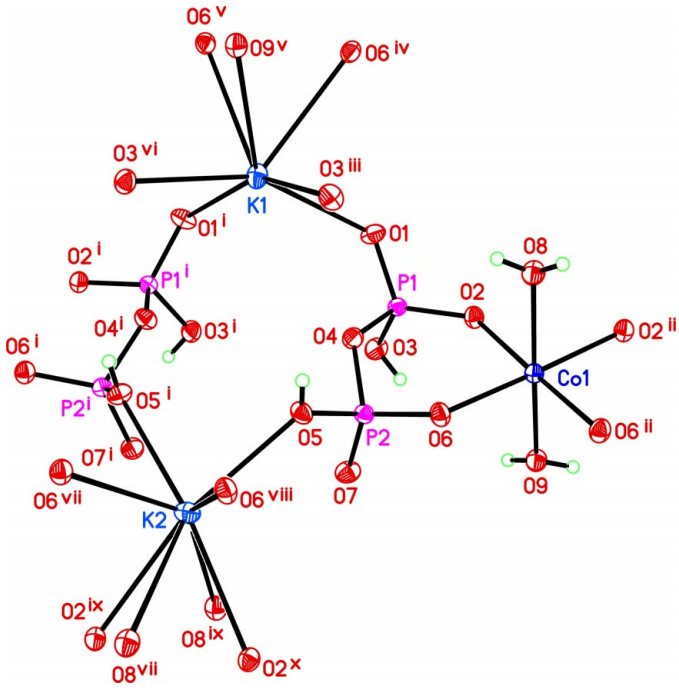

Figure 1
Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level. Symmetry operators for generating equivalent atoms: (i) $x,\frac{1}{2}-y,z$; (ii) $x,\frac{3}{2}-y,z$; (iii) $\frac{1}{2}+x,y,\frac{1}{2}-z$; (iv) $-\frac{1}{2}+x,1-y,-\frac{1}{2}+z$; (v) $\frac{1}{2}-x,-\frac{1}{2}+y,-\frac{1}{2}+z$; (vi) $-\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}-z$; (vii) $-x,-\frac{1}{2}+y,1-z$; (viii) $-x,1-y,1-z$; (ix) $\frac{1}{2}-x,-\frac{1}{2}+y,\frac{1}{2}+z$; (x) $\frac{1}{2}-x,1-y,\frac{1}{2}+z$.

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