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Bis(2,6-dimethylanilinium) diaquabis-(dihydrogen diphosphato- κ^2O,O')-cobaltate(II)

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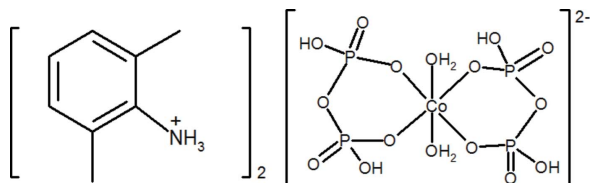
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(C-C) = 0.005$ Å; R factor = 0.061; wR factor = 0.168; data-to-parameter ratio = 35.4.

In the title compound, $(C_8H_{12}N)_2[Co(H_2P_2O_7)_2(H_2O)_2]$, the Co^{2+} ion lies on a crystallographic inversion centre and adopts a slightly distorted octahedral CoO_6 coordination geometry arising from two chelating diphosphate $[H_2P_2O_7]^{2-}$ ligands and two *trans* water molecules. In the crystal, the components are linked by $O-H\cdots O$, $N-H\cdots O$ and $C-H\cdots O$ hydrogen bonds and weak aromatic $\pi-\pi$ stacking [shortest centroid-centroid separation = 3.778 (2) Å] interactions. (001) layers of alternating organic cations and complex inorganic anions are apparent.

Related literature

For related structures, see: Ahmed *et al.* (2006); Selmi *et al.* (2006, 2009); Gharbi *et al.* (1994); Gharbi & Jouini (2004); Elboulali *et al.* (2013a,b); Essehli *et al.* (2006).



Experimental

Crystal data

 $(C_8H_{12}N)_2[Co(H_2P_2O_7)_2(H_2O)_2]$ $M_r = 691.25$ Triclinic, $P\bar{1}$ $a = 7.320$ (3) Å $b = 7.584$ (4) Å $c = 13.413$ (2) Å $\alpha = 85.35$ (3)° $\beta = 75.56$ (2)° $\gamma = 74.42$ (5)° $V = 694.5$ (5) Å³ $Z = 1$ Ag $K\alpha$ radiation $\lambda = 0.56087$ Å $\mu = 0.48$ mm⁻¹ $T = 293$ K

0.40 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
 $T_{\min} = 0.799$, $T_{\max} = 0.982$
9085 measured reflections

6683 independent reflections
5514 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.080$
2 standard reflections every 120 min
intensity decay: 5%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.061$
 $wR(F^2) = 0.168$
 $S = 1.04$
6683 reflections
189 parameters
3 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 1.57$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.82$ e Å⁻³

Table 1

Selected bond lengths (Å).

Co1—O5	2.0645 (18)	Co1—O1W	2.130 (2)
Co1—O1	2.0744 (17)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2—H2 \cdots O6 ⁱ	0.82	1.72	2.532 (3)	174
O7—H7 \cdots O3 ⁱⁱ	0.82	1.70	2.505 (3)	167
O1W—H2W1 \cdots O4 ⁱ	0.87 (2)	2.11 (2)	2.947 (3)	161 (4)
O1W—H1W1 \cdots O7 ⁱⁱⁱ	0.86 (2)	1.96 (2)	2.813 (3)	177 (4)
N1—H1C \cdots O6 ^{iv}	0.89	1.94	2.828 (3)	175
N1—H1A \cdots O3 ⁱⁱ	0.89	1.93	2.805 (3)	168
N1—H1B \cdots O5	0.89	2.29	3.005 (3)	138
N1—H1B \cdots O1 ^v	0.89	2.37	3.016 (3)	129
C7—H7C \cdots O2 ⁱⁱ	0.96	2.58	3.497 (5)	160
C7—H7A \cdots O6 ^{iv}	0.96	2.57	3.343 (4)	138

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7194).

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supporting information

Acta Cryst. (2014). E70, m86–m87 [doi:10.1107/S1600536814002530]

Bis(2,6-dimethylanilinium) diaquabis(dihydrogen diphosphato- κ^2O,O')cobaltate(II)

Ahlem Ben Saad, Ahmed Selmi, Mohamed Rzaigui and Samah Toumi Akriche

S1. Comment

The present work is a part of our investigation of diphosphate materials of mixed organic-metal cations. Here, we report a new synthesized one: $(C_8H_{12}N)_2[Co(H_2P_2O_7)_2(H_2O)_2]^{2-}$ (I).

The asymmetric unit of (I) is made up of a half of mononuclear $[Co(H_2P_2O_7)_2(H_2O)_2]^{2-}$ moiety and one of 2,6-xylylidinium cation. As Co^{2+} ion lie on inversion centre, the complete formula unit is generated by this element of symmetry (Fig. 1).

The inorganic component is made up of anionic monomeric units of formula $[Co(H_2P_2O_7)_2(H_2O)_2]^{2-}$, in which the six-coordinated cobalt (II) ions are linked by means of $O-H\cdots O$ (with $2.505(3) \text{ \AA} < O\cdots O < 2.947(3) \text{ \AA}$ see Table 1) hydrogen bonds to develop anionic layers running perpendicular to c axis. Similar $[M(H_2P_2O_7)_2(H_2O)_2]^{2-}$ two-dimensional topological framework can be also found in the previously reported diphosphate materials (Selmi *et al.*, 2006, 2009; Elboulali *et al.*, 2013*a,b*). The cobalt (II) complex adopts a distorted octahedral where the four O atoms of diphosphate bidentate ligand (O1, O5, O1ⁱ and O5ⁱ with (i); $-x + 1, -y + 1, -z + 1$) fill the equatorial positions and the two symmetry equivalent O atoms of water molecules (O1W, O1Wⁱ with (i); $-x + 1, -y + 1, -z + 1$) occupy the apical ones. The bond distances and angles in CoO_6 are sufficiently close to those found in the related $M^II O_6$ complexes featuring the chelating diphosphate ligand (Ahmed *et al.*, 2006; Elboulali *et al.*, 2013*a*, 2013*b*; Essehli *et al.*, 2006; Gharbi *et al.*, 1994; Gharbi *et al.*, 2004; Selmi *et al.*, 2006 and 2009).

Two phosphorous atoms are tetrahedrally coordinated and covalently linked through O4 to form a P_2O_7 group with bent geometry ($P1-O4-P2 = 129.66(12)^\circ$) and quasi-eclipsed conformation as confirmed by the torsion angle values 11.66° , 5.76° and 7.16° respectively of $O5-P2-P1-O1$, $O7-P2-P1-O3$ and $O6-P2-P1-O2$.

In the crystal of 1, the 2,6-xylylidinium cations are linked by means $N-H\cdots O$ and $C-H\cdots O$ hydrogen bonds to inorganic layers thanks to NH_3 group of the protonated cations (Fig. 2). It's to be noted that two adjacent cations interact by weak $\pi\cdots\pi$ stacking interactions (values of the inter-planar distances of $3.778(2) \text{ \AA}$).

S2. Experimental

Pink blocks of the title compound were grown at room temperature by slow evaporation from water-ethanol (80/20) solution containing a stoichiometric mixture of $CoCl_2 \cdot 6H_2O$ (0.12 mg, 0.5 mmol), 2,6-xylylidine (0.12 mL, 1 mmol) and $N_4P_2O_7 \cdot 10H_2O$ (0.45 mg, 1 mmol) dissolved in 2 ml of hydrochloric acid solution (2M).

S3. Refinement

Due to poor quality of the crystal when being diffracted, some bad reflections (with $(I_{obs}-I_{calc})/\sigma I_{obs} > 10$) are observed. For the final refinement they are omitted. H atoms attached to C, O and N atoms were fixed geometrically and treated as riding, with $C-H = 0.93 \text{ \AA}$ with $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic ring and $C-H = 0.96 \text{ \AA}$ and $N-H = 0.89 \text{ \AA}$ respectively for CH_3 and NH_3 cation radicals and $O-H = 0.82 \text{ \AA}$ for diphosphoric anion with $U_{iso}(H) = 1.5U_{eq}(C, O)$ or

N). The water H atoms were refined using restraints [$O-H = 0.85$ (1) Å, $H\cdots H = 1.44$ (2) Å and $U_{iso}(H) = 1.5U_{eq}(O)$].

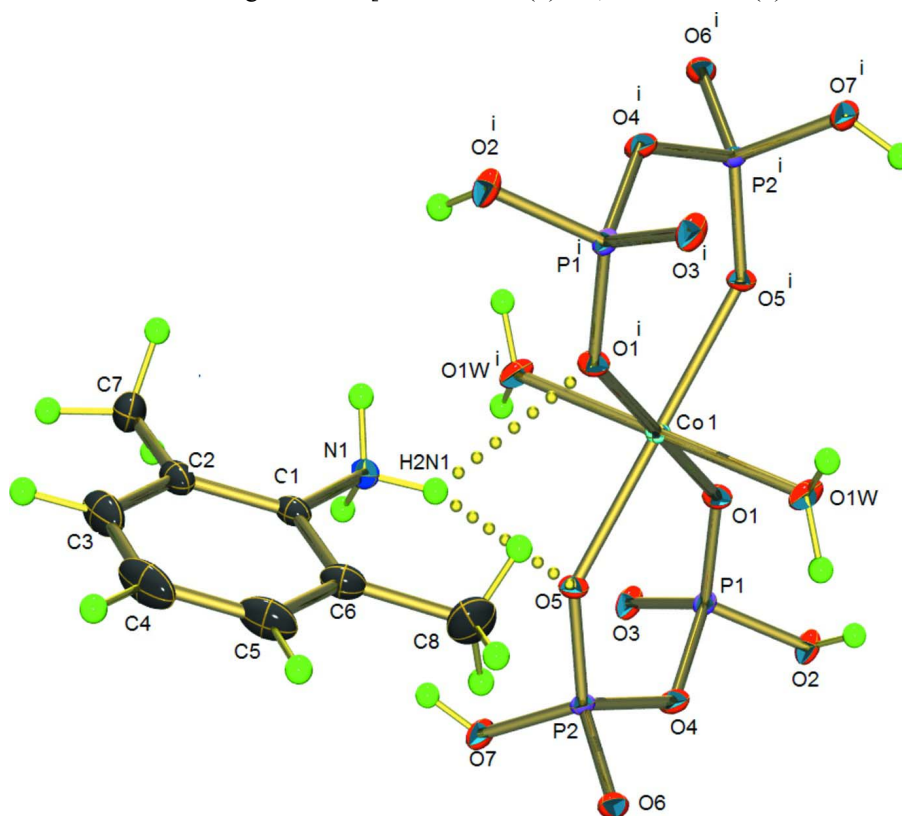


Figure 1

An *ORTEP* view of (I) with displacement ellipsoids drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii. Hydrogen bonds are represented as dashed lines. [Symmetry code: (i) $1 - x, 1 - y, 1 - z$.]

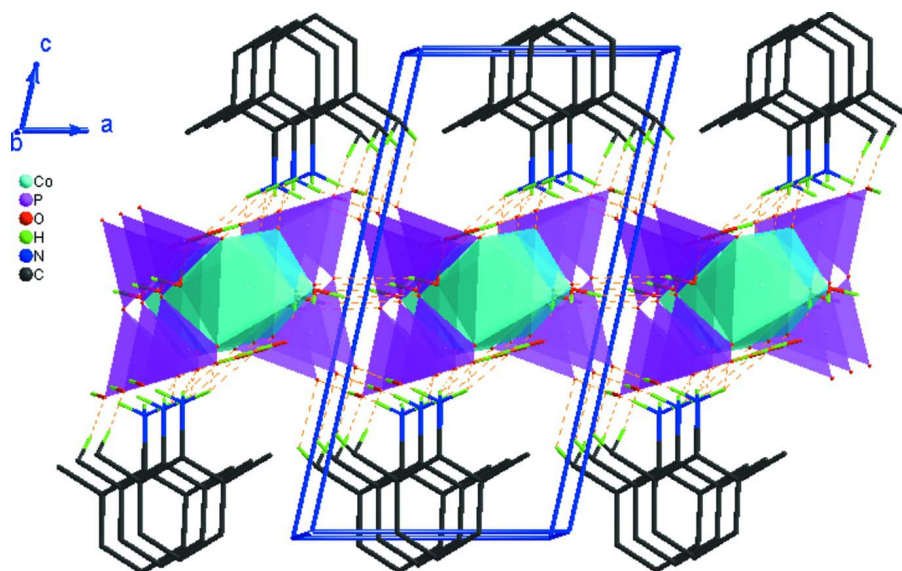


Figure 2

Perspective view of crystal packing of (I). The H-atoms not involved in H-bonding are omitted.

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Crystal data

 $(C_8H_{12}N)_2[Co(H_2P_2O_7)_2(H_2O)_2]$ $M_r = 691.25$ Triclinic, $P\bar{1}$ $a = 7.320$ (3) Å $b = 7.584$ (4) Å $c = 13.413$ (2) Å $\alpha = 85.35$ (3)° $\beta = 75.56$ (2)° $\gamma = 74.42$ (5)° $V = 694.5$ (5) Å³ $Z = 1$ $F(000) = 357$ $D_x = 1.653$ Mg m⁻³Ag $K\alpha$ radiation, $\lambda = 0.56087$ Å

Cell parameters from 25 reflections

 $\theta = 9\text{--}11^\circ$ $\mu = 0.48$ mm⁻¹ $T = 293$ K

Prism, pink

 $0.40 \times 0.30 \times 0.20$ mm

Data collection

Enraf–Nonius CAD-4
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

non-profiled ω scansAbsorption correction: ψ scan
(North *et al.*, 1968) $T_{\min} = 0.799$, $T_{\max} = 0.982$

9085 measured reflections

6683 independent reflections

5514 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.080$ $\theta_{\max} = 28.0^\circ$, $\theta_{\min} = 2.2^\circ$ $h = -12 \rightarrow 12$ $k = -12 \rightarrow 12$ $l = -5 \rightarrow 22$

2 standard reflections every 120 min

intensity decay: 5%

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.061$ $wR(F^2) = 0.168$ $S = 1.04$

6683 reflections

189 parameters

3 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sitesH atoms treated by a mixture of independent
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.0826P)^2 + 0.9452P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.005$ $\Delta\rho_{\max} = 1.57$ e Å⁻³ $\Delta\rho_{\min} = -0.82$ e Å⁻³

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.5000	0.5000	0.5000	0.01796 (9)
P1	0.69129 (7)	0.72084 (7)	0.63065 (4)	0.01948 (10)

P2	0.80524 (7)	0.75466 (7)	0.40670 (4)	0.01867 (10)
O1	0.5727 (2)	0.5931 (2)	0.62242 (13)	0.0242 (3)
O2	0.8322 (3)	0.6463 (2)	0.70245 (15)	0.0287 (3)
H2	0.8794	0.5361	0.6937	0.043*
O3	0.5808 (3)	0.9121 (2)	0.66208 (16)	0.0306 (4)
O4	0.8430 (2)	0.7284 (3)	0.52092 (14)	0.0274 (3)
O5	0.6535 (2)	0.6611 (2)	0.40048 (13)	0.0245 (3)
O6	1.0029 (2)	0.6880 (2)	0.33643 (15)	0.0281 (3)
O7	0.7321 (3)	0.9654 (2)	0.39394 (17)	0.0308 (4)
H7	0.6270	0.9903	0.3778	0.046*
O1W	0.7487 (2)	0.2730 (2)	0.49181 (18)	0.0327 (4)
H1W1	0.748 (6)	0.178 (4)	0.462 (3)	0.049*
H2W1	0.865 (4)	0.291 (5)	0.477 (3)	0.049*
N1	0.3681 (3)	0.7717 (3)	0.26576 (15)	0.0258 (3)
H1A	0.3675	0.8804	0.2865	0.039*
H1B	0.4577	0.6849	0.2885	0.039*
H1C	0.2511	0.7508	0.2908	0.039*
C1	0.4143 (4)	0.7700 (4)	0.15241 (18)	0.0291 (4)
C2	0.2798 (5)	0.8852 (4)	0.1038 (2)	0.0367 (5)
C3	0.3238 (7)	0.8820 (6)	-0.0032 (3)	0.0530 (9)
H3	0.2364	0.9570	-0.0382	0.064*
C4	0.4949 (8)	0.7695 (7)	-0.0583 (2)	0.0616 (12)
H4	0.5210	0.7680	-0.1298	0.074*
C5	0.6260 (6)	0.6602 (6)	-0.0078 (2)	0.0540 (10)
H5	0.7416	0.5865	-0.0457	0.065*
C6	0.5902 (5)	0.6569 (4)	0.0994 (2)	0.0378 (6)
C7	0.0963 (5)	1.0126 (5)	0.1621 (3)	0.0477 (7)
H7A	0.0077	0.9431	0.1985	0.072*
H7B	0.0364	1.0961	0.1147	0.072*
H7C	0.1273	1.0802	0.2102	0.072*
C8	0.7374 (5)	0.5355 (6)	0.1532 (3)	0.0556 (9)
H8A	0.8042	0.6090	0.1783	0.083*
H8B	0.8302	0.4477	0.1057	0.083*
H8C	0.6715	0.4726	0.2100	0.083*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01549 (15)	0.01757 (15)	0.02352 (17)	-0.00720 (11)	-0.00640 (12)	-0.00003 (12)
P1	0.0174 (2)	0.01835 (19)	0.0248 (2)	-0.00437 (15)	-0.00820 (16)	-0.00249 (16)
P2	0.01319 (18)	0.01767 (19)	0.0260 (2)	-0.00567 (14)	-0.00438 (15)	-0.00018 (16)
O1	0.0256 (7)	0.0265 (7)	0.0252 (7)	-0.0133 (5)	-0.0071 (5)	-0.0016 (5)
O2	0.0286 (7)	0.0271 (7)	0.0330 (8)	-0.0007 (6)	-0.0171 (6)	-0.0051 (6)
O3	0.0286 (7)	0.0206 (6)	0.0450 (10)	-0.0003 (6)	-0.0174 (7)	-0.0082 (6)
O4	0.0206 (6)	0.0389 (8)	0.0276 (7)	-0.0137 (6)	-0.0087 (5)	0.0010 (6)
O5	0.0236 (6)	0.0279 (7)	0.0279 (7)	-0.0154 (5)	-0.0083 (5)	0.0032 (5)
O6	0.0176 (6)	0.0248 (7)	0.0369 (9)	-0.0044 (5)	0.0010 (6)	0.0012 (6)
O7	0.0235 (7)	0.0185 (6)	0.0539 (11)	-0.0040 (5)	-0.0166 (7)	-0.0014 (6)

O1W	0.0191 (6)	0.0259 (7)	0.0549 (12)	-0.0031 (6)	-0.0118 (7)	-0.0099 (7)
N1	0.0265 (8)	0.0297 (8)	0.0232 (8)	-0.0104 (7)	-0.0062 (6)	0.0003 (6)
C1	0.0362 (11)	0.0345 (10)	0.0227 (9)	-0.0204 (9)	-0.0061 (8)	0.0002 (8)
C2	0.0475 (14)	0.0433 (13)	0.0310 (11)	-0.0272 (12)	-0.0166 (10)	0.0089 (10)
C3	0.078 (3)	0.068 (2)	0.0340 (14)	-0.045 (2)	-0.0286 (16)	0.0146 (14)
C4	0.099 (3)	0.080 (3)	0.0228 (12)	-0.057 (3)	-0.0082 (16)	0.0011 (14)
C5	0.070 (2)	0.065 (2)	0.0286 (13)	-0.0376 (19)	0.0110 (14)	-0.0132 (13)
C6	0.0413 (13)	0.0433 (13)	0.0295 (11)	-0.0205 (11)	0.0030 (10)	-0.0084 (10)
C7	0.0455 (16)	0.0484 (17)	0.0554 (19)	-0.0149 (13)	-0.0249 (15)	0.0147 (14)
C8	0.0376 (15)	0.061 (2)	0.057 (2)	-0.0017 (15)	0.0009 (14)	-0.0131 (17)

Geometric parameters (Å, °)

Co1—O5 ⁱ	2.0645 (18)	N1—H1B	0.8900
Co1—O5	2.0645 (18)	N1—H1C	0.8900
Co1—O1	2.0744 (17)	C1—C2	1.386 (4)
Co1—O1 ⁱ	2.0744 (17)	C1—C6	1.396 (4)
Co1—O1W ⁱ	2.130 (2)	C2—C3	1.391 (4)
Co1—O1W	2.130 (2)	C2—C7	1.500 (5)
P1—O1	1.4905 (17)	C3—C4	1.383 (7)
P1—O3	1.495 (2)	C3—H3	0.9300
P1—O2	1.5505 (18)	C4—C5	1.369 (7)
P1—O4	1.6151 (19)	C4—H4	0.9300
P2—O5	1.4910 (17)	C5—C6	1.395 (4)
P2—O6	1.4971 (18)	C5—H5	0.9300
P2—O7	1.5529 (19)	C6—C8	1.509 (6)
P2—O4	1.6110 (19)	C7—H7A	0.9600
O2—H2	0.8200	C7—H7B	0.9600
O7—H7	0.8200	C7—H7C	0.9600
O1W—H1W1	0.856 (18)	C8—H8A	0.9600
O1W—H2W1	0.867 (18)	C8—H8B	0.9600
N1—C1	1.473 (3)	C8—H8C	0.9600
N1—H1A	0.8900		
O5 ⁱ —Co1—O5	180.0	C1—N1—H1B	109.5
O5 ⁱ —Co1—O1	90.34 (7)	H1A—N1—H1B	109.5
O5—Co1—O1	89.66 (7)	C1—N1—H1C	109.5
O5 ⁱ —Co1—O1 ⁱ	89.66 (7)	H1A—N1—H1C	109.5
O5—Co1—O1 ⁱ	90.34 (7)	H1B—N1—H1C	109.5
O1—Co1—O1 ⁱ	180.0	C2—C1—C6	123.4 (3)
O5 ⁱ —Co1—O1W ⁱ	93.83 (8)	C2—C1—N1	117.4 (2)
O5—Co1—O1W ⁱ	86.17 (8)	C6—C1—N1	119.2 (2)
O1—Co1—O1W ⁱ	92.18 (8)	C1—C2—C3	117.1 (3)
O1 ⁱ —Co1—O1W ⁱ	87.82 (8)	C1—C2—C7	122.5 (3)
O5 ⁱ —Co1—O1W	86.17 (8)	C3—C2—C7	120.4 (3)
O5—Co1—O1W	93.83 (8)	C4—C3—C2	121.2 (4)
O1—Co1—O1W	87.82 (8)	C4—C3—H3	119.4
O1 ⁱ —Co1—O1W	92.18 (8)	C2—C3—H3	119.4

O1W ⁱ —Co1—O1W	180.0	C5—C4—C3	120.0 (3)
O1—P1—O3	116.44 (11)	C5—C4—H4	120.0
O1—P1—O2	112.85 (11)	C3—C4—H4	120.0
O3—P1—O2	107.98 (11)	C4—C5—C6	121.5 (4)
O1—P1—O4	108.32 (10)	C4—C5—H5	119.2
O3—P1—O4	108.67 (12)	C6—C5—H5	119.2
O2—P1—O4	101.45 (10)	C5—C6—C1	116.8 (3)
O5—P2—O6	116.77 (11)	C5—C6—C8	120.5 (3)
O5—P2—O7	111.33 (10)	C1—C6—C8	122.8 (3)
O6—P2—O7	109.58 (11)	C2—C7—H7A	109.5
O5—P2—O4	109.55 (9)	C2—C7—H7B	109.5
O6—P2—O4	104.85 (10)	H7A—C7—H7B	109.5
O7—P2—O4	103.77 (11)	C2—C7—H7C	109.5
P1—O1—Co1	133.68 (10)	H7A—C7—H7C	109.5
P1—O2—H2	109.5	H7B—C7—H7C	109.5
P2—O4—P1	129.66 (11)	C6—C8—H8A	109.5
P2—O5—Co1	134.76 (11)	C6—C8—H8B	109.5
P2—O7—H7	109.5	H8A—C8—H8B	109.5
Co1—O1W—H1W1	116 (3)	C6—C8—H8C	109.5
Co1—O1W—H2W1	120 (3)	H8A—C8—H8C	109.5
H1W1—O1W—H2W1	111 (3)	H8B—C8—H8C	109.5
C1—N1—H1A	109.5		
O3—P1—O1—Co1	99.39 (16)	O1—Co1—O5—P2	17.64 (15)
O2—P1—O1—Co1	-134.89 (14)	O1 ⁱ —Co1—O5—P2	-162.36 (15)
O4—P1—O1—Co1	-23.38 (17)	O1W ⁱ —Co1—O5—P2	109.84 (16)
O5 ⁱ —Co1—O1—P1	178.85 (15)	O1W—Co1—O5—P2	-70.16 (16)
O5—Co1—O1—P1	-1.15 (15)	C6—C1—C2—C3	1.6 (4)
O1 ⁱ —Co1—O1—P1	10 (100)	N1—C1—C2—C3	-179.6 (2)
O1W ⁱ —Co1—O1—P1	-87.30 (15)	C6—C1—C2—C7	-176.8 (3)
O1W—Co1—O1—P1	92.70 (15)	N1—C1—C2—C7	2.0 (4)
O5—P2—O4—P1	-35.28 (19)	C1—C2—C3—C4	-0.4 (5)
O6—P2—O4—P1	-161.35 (15)	C7—C2—C3—C4	178.1 (3)
O7—P2—O4—P1	83.69 (17)	C2—C3—C4—C5	-0.9 (6)
O1—P1—O4—P2	47.67 (18)	C3—C4—C5—C6	1.0 (6)
O3—P1—O4—P2	-79.70 (17)	C4—C5—C6—C1	0.1 (5)
O2—P1—O4—P2	166.66 (15)	C4—C5—C6—C8	-179.8 (4)
O6—P2—O5—Co1	114.85 (16)	C2—C1—C6—C5	-1.5 (4)
O7—P2—O5—Co1	-118.29 (16)	N1—C1—C6—C5	179.7 (2)
O4—P2—O5—Co1	-4.09 (18)	C2—C1—C6—C8	178.5 (3)
O5 ⁱ —Co1—O5—P2	-89 (100)	N1—C1—C6—C8	-0.3 (4)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O2—H2 \cdots O6 ⁱⁱ	0.82	1.72	2.532 (3)	174

O7—H7…O3 ⁱⁱⁱ	0.82	1.70	2.505 (3)	167
O1 <i>W</i> —H2 <i>W</i> 1…O4 ⁱⁱ	0.87 (2)	2.11 (2)	2.947 (3)	161 (4)
O1 <i>W</i> —H1 <i>W</i> 1…O7 ^{iv}	0.86 (2)	1.96 (2)	2.813 (3)	177 (4)
N1—H1C…O6 ^v	0.89	1.94	2.828 (3)	175
N1—H1A…O3 ⁱⁱⁱ	0.89	1.93	2.805 (3)	168
N1—H1B…O5	0.89	2.29	3.005 (3)	138
N1—H1B…O1 ⁱ	0.89	2.37	3.016 (3)	129
C7—H7C…O2 ⁱⁱⁱ	0.96	2.58	3.497 (5)	160
C7—H7A…O6 ^v	0.96	2.57	3.343 (4)	138

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