Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[diquinolinium [[diaquacobaltate(II)]-μ-cyclotetraphosphato] hexahydrate]

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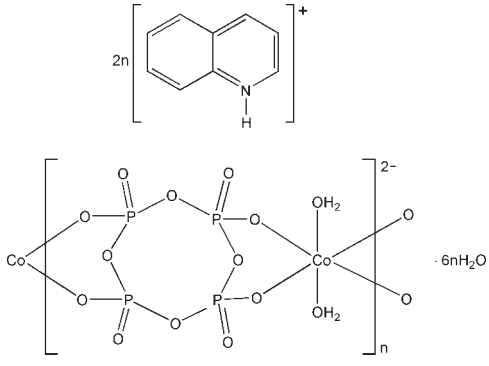
Received 9 January 2010; accepted 17 January 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.057; wR factor = 0.164; data-to-parameter ratio = 30.6.

The cyclotetraphosphate anion, $[P_4O_{12}]^{4-}$, forms the title complex with cobalt(II) and quinolinium, $\{(C_9H_8N)_2[Co(P_4O_{12})(H_2O)_2]\cdot 6H_2O\}_n$. In the complex anion, the Co^{II} ion, lying on an inversion center, is surrounded by four phosphate O atoms and two water molecules in a slightly distorted octahedral geometry. The crystal structure consists of anionic ribbons of formula $\{[Co(P_4O_{12})(H_2O)_2]^{2-}\}_n$ extending along [100]. A network of O—H···O, N—H···O and C—H···O hydrogen bonds consolidates the crystal packing.

Related literature

For the crystal chemistry of condensed phosphates, see: Durif (1995). For general background to transition metal–organic derivatives of polyoxoanions, see: Feher & Budzichowski (1995); Guerrero *et al.* (1999); Ikotun *et al.* (2008); Lugmair & Tilley (1998). For general background to hydrogen bonds, see: Blessing (1986); Brown (1976); Steiner & Saenger (1993). For the synthesis, see: Ondik (1964).



Experimental

Crystal data

$(C_9H_8N)_2[Co(P_4O_{12})(H_2O)_2]\cdot 6H_2O$
M_r = 779.27
Triclinic, $P\overline{1}$
a = 7.443 (3) Å
b = 10.037 (4) Å
c = 10.682 (7) Å
α = 83.74 (4)°
β = 70.98 (4)°
γ = 85.71 (3)°
V = 749.4 (6) Å^3
Z = 1
Ag $K\alpha$ radiation
λ = 0.56083 Å
μ = 0.46 mm^{-1}
T = 293 K
0.20 × 0.18 × 0.16 mm

Data collection

Enraf–Nonius TurboCAD-4 diffractometer
12878 measured reflections
7242 independent reflections
4531 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
2 standard reflections every 120 min
intensity decay: 2%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.164
S = 0.98
7242 reflections
237 parameters
13 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.11 e Å^{-3}
$\Delta\rho_{min}$ = −1.46 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2	0.86	1.88	2.728 (3)	171
O1—H11···O4	0.83 (3)	1.98 (3)	2.747 (3)	154 (3)
O1—H21···O2^{i}	0.84 (3)	2.00 (3)	2.841 (3)	179 (4)
O2—H12···O3^{ii}	0.83 (3)	1.85 (3)	2.666 (3)	168 (3)
O2—H22···O6	0.83 (3)	1.95 (3)	2.771 (3)	172 (4)
O3—H13···O6	0.86 (2)	1.95 (2)	2.743 (3)	152 (3)
O3—H23···O5^{iii}	0.87 (3)	2.02 (2)	2.833 (3)	154 (3)
O4—H14···O9^{iv}	0.86 (2)	2.01 (2)	2.824 (3)	157 (4)
O4—H24···O9^{i}	0.86 (3)	2.06 (3)	2.890 (3)	163 (3)
C7—H7···O9^{v}	0.93	2.59	3.459 (4)	156
C9—H9···O3	0.93	2.54	3.080 (4)	118
C9—H9···O10^{vi}	0.93	2.59	3.381 (3)	143

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+3, -y+1, -z$; (iii) $-x+2, -y+1, -z$; (iv) $-x+1, -y+2, -z+1$; (v) $-x+2, -y+2, -z$; (vi) $x+1, y, z-1$.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1989); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2272).

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supporting information

Acta Cryst. (2010). E**66**, m186–m187 [https://doi.org/10.1107/S1600536810002096]

catena-Poly[diquinolinium [[diaquacobaltate(II)]-μ-cyclotetraphosphato] hexahydrate]

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S1. Comment

Transition metal–organic derivatives of polyoxoanions have recently been attracting considerable attention, because they serve as molecular models of metal species bound on oxo surfaces of heterogeneous catalysts (Feher & Budzichowski, 1995). In this context, several frameworks of this kind of materials with one-, two- or three-dimensional networks have been successfully constructed by using monophosphates, monophosphonates and monophosphinates (Guerrero *et al.*, 1999; Lugmair & Tilley, 1998). In contrast, structural diversity of transition metal–organic derivatives of condensed phosphates has been much less explored. In order to enrich the varieties in such kinds of hybrid materials, we report the synthesis and crystal structure of $(C_9H_8N)_2[Co(P_4O_{12})(H_2O)_2].6H_2O$.

The title compound contains protonated quinolinium cations, diaquacyclotetraphosphatocobaltate(II) dianions and water molecules (Fig. 1). The cyclic phosphate anion, $[P_4O_{12}]^{4-}$, is located around an inversion center and so is built up by only two independent PO_4 tetrahedra. Its main geometrical features [the bond lengths P—O = 1.473 (2)–1.603 (2) Å, and the bond angles O—P—O = 100.24 (9)–121.11 (1)°, P—O—P = 134.40 (1)–137.25 (1)°] are not significantly different from what is commonly observed in other cyclotetraphosphate anions with the same internal symmetry (Durif, 1995). The coordination polyhedron of the Co^{II} atom, which lies on an inversion center, is octahedral with four external O atoms O(E) from two adjacent bidentate cyclotetraphosphates and two water O atoms O(w), providing a Co atom with six O donor set [four O(E) equatorial arrangement with two axial O(w)]. The Co—O bond lengths fall within the range of 2.106 (2)–2.116 (2) Å. The shortest distance between two neighboring Co atoms is 7.443 (3) Å. This distance could explain the cobalt magnetic properties in several materials (Ikotun *et al.*, 2008). The $[CoO_4(H_2O)_2]$ octahedra alternate with the P_4O_{12} rings as to form infinite ribbons, fused through Co—O—P linkage, propagating along the *a* axis (Fig. 2). The protonated quinolinim is located in the inter-ribbons spacing, and it neutralizes the negative charge of the anionic part. These organic entities are planar as evidenced by the mean deviation (±0.005 Å) from least square plane defined by the nine constituent atoms. As well as electrostatic and van der Waals interactions, the component species of the title compound establish a three-dimensional network through N—H···O and O—H···O hydrogen bonds. The structure is further stabilized with non-classical hydrogen bonds of the C—H···O type (Steiner & Saenger, 1993). The examination of the hydrogen-bond scheme shows that hydrogen bond connecting C9 to the phosphate group and water molecule is bifurcated. In the structure, there are two strong hydrogen bonds, with O···O distances of 2.666 (3) and 2.728 (3) Å. The others are weaker, with O(N, C)···O ranging from 2.743 (3) to 3.459 (4) Å (Blessing, 1986; Brown, 1976).

S2. Experimental

The title compound was prepared by adding ethanolic solution (5 ml) of quinoline (8.34 mmol) dropwise to a mixture of $H_4P_4O_{12}$ (4.15 mmol) and $CoCl_2$ (4.15 mmol) in water (20 ml). Pink prism crystals of good quality were obtained after a slow evaporation during few days at ambient temperature. The cyclotetraphosphoric acid, $H_4P_4O_{12}$, was produced from

$Na_4P_4O_{12}.4H_2O$, prepared according to the Ondik process (Ondik, 1964) through an ion-exchange resin in H-state (Amberlite IR 120).

S3. Refinement

H atoms on C and N atoms were positioned geometrically and treated as riding on their parent atoms, with N—H = 0.86, C—H =0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C,N). H atoms of water molecules were located from difference Fourier maps and refined isotropically. The highest residual electron density was found 0.73 Å from Co1 and the deepest hole 0.76 Å from Co1.

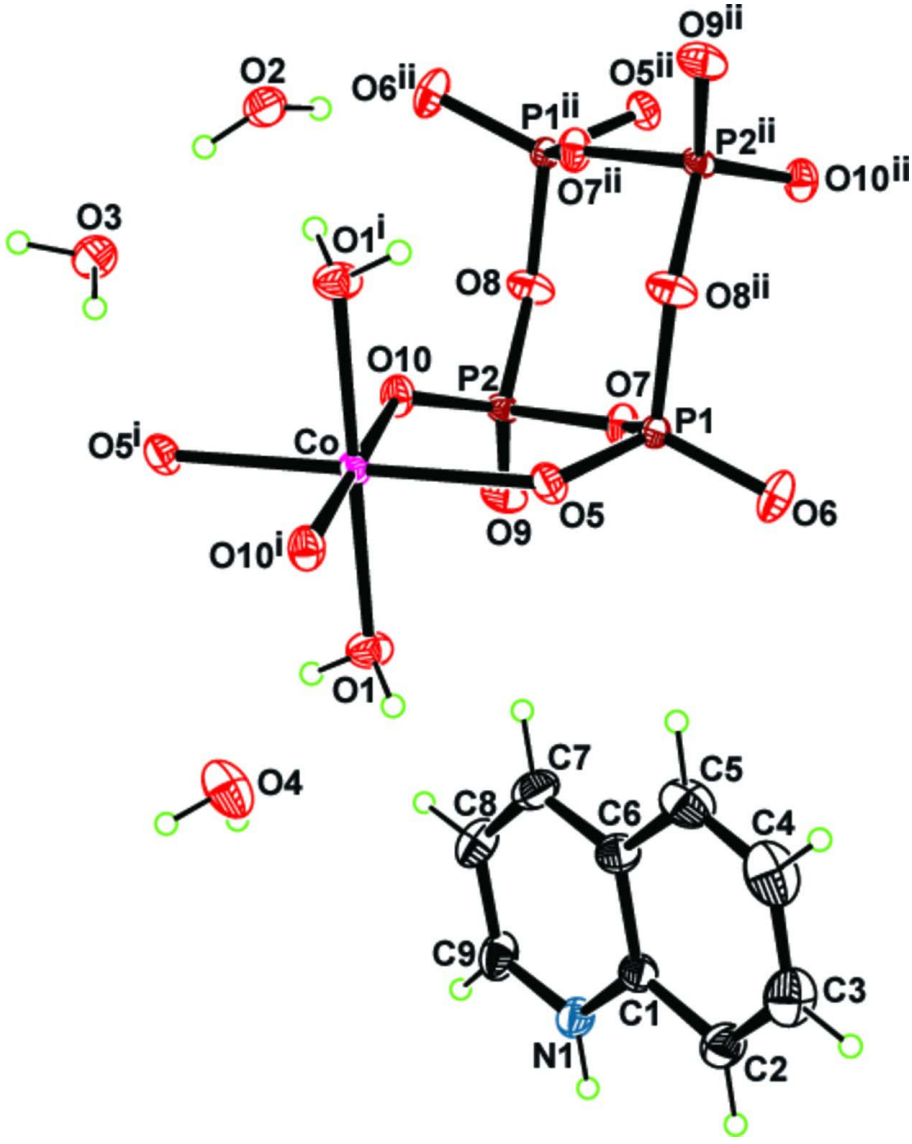

Figure 1

The structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) 1-x, 1-y, 1-z; (ii) 2-x, 1-y, 1-z.]

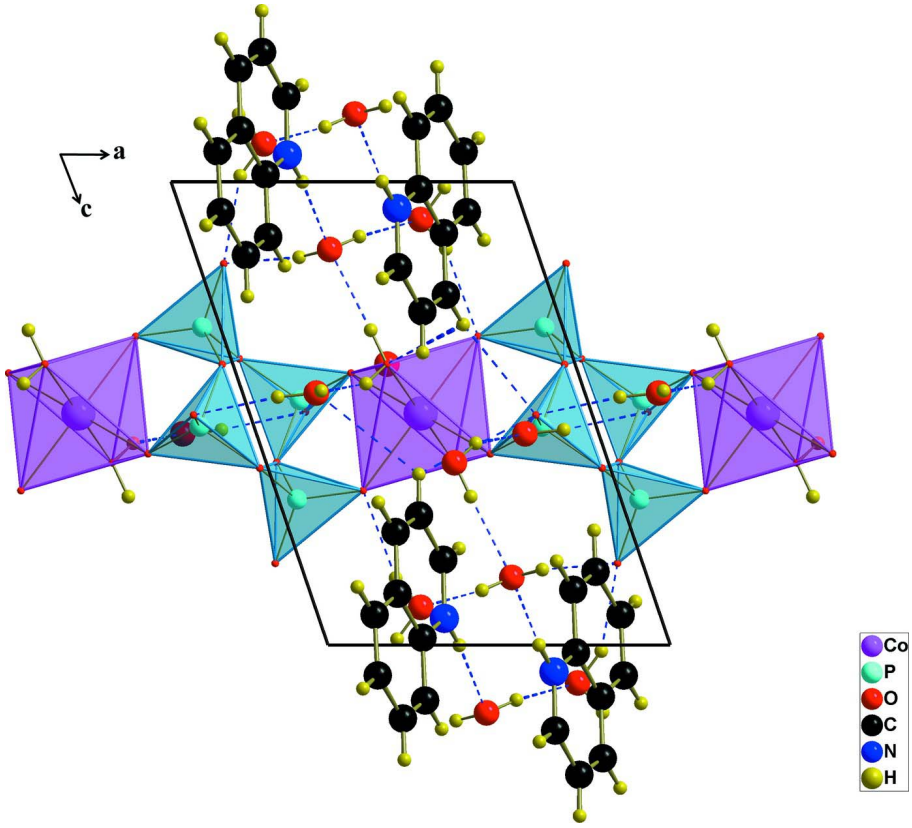

Figure 2

Projection of the title compound along the *b* axis.

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Crystal data

$(C_9H_8N)_2[Co(P_4O_{12})(H_2O)_2]\cdot 6H_2O$
$M_r = 779.27$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.443$ (3) Å
$b = 10.037$ (4) Å
$c = 10.682$ (7) Å
$\alpha = 83.74$ (4)°
$\beta = 70.98$ (4)°
$\gamma = 85.71$ (3)°
$V = 749.4$ (6) Å^3
$Z = 1$
$F(000) = 401$
$D_x = 1.727$ Mg m^{-3}
Ag $K\alpha$ radiation, $\lambda = 0.56083$ Å
Cell parameters from 25 reflections
$\theta = 9.0$–$11.0°$
$\mu = 0.46$ mm^{-1}
$T = 293$ K
Prism, pink
0.20 × 0.18 × 0.16 mm

Data collection

Enraf–Nonius TurboCAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
non–profiled $\omega/2\theta$ scans
12878 measured reflections
7242 independent reflections
4531 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 28.0°$, $\theta_{min} = 2.2°$
$h = -12 \rightarrow 12$
$k = -16 \rightarrow 16$
$l = -17 \rightarrow 10$
2 standard reflections every 120 min
intensity decay: 2%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.164$
$S = 0.98$
7242 reflections
237 parameters
13 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.097P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.022$
$\Delta\rho_{max} = 1.11$ e Å^{-3}
$\Delta\rho_{min} = -1.46$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.5000	0.5000	0.5000	0.02117 (10)
P2	0.84035 (7)	0.67186 (5)	0.52866 (5)	0.02037 (11)
P1	0.94639 (7)	0.49127 (5)	0.31420 (5)	0.02082 (11)
O5	0.7442 (2)	0.47075 (18)	0.33361 (17)	0.0290 (3)
O9	0.8351 (3)	0.81917 (16)	0.5033 (2)	0.0353 (4)
O8	0.9759 (3)	0.63833 (17)	0.6180 (2)	0.0329 (4)
O7	0.9688 (2)	0.61035 (16)	0.39418 (17)	0.0284 (3)
O1	0.4503 (3)	0.68127 (18)	0.39353 (19)	0.0348 (4)
O6	1.0732 (3)	0.5182 (2)	0.17668 (18)	0.0410 (4)
C1	1.2832 (4)	0.9562 (2)	−0.0159 (3)	0.0314 (4)
N1	1.3663 (3)	0.8353 (2)	−0.0577 (2)	0.0350 (4)
H1	1.3836	0.7736	0.0002	0.042*
C2	1.2288 (5)	0.9765 (3)	0.1194 (3)	0.0432 (6)
H2	1.2488	0.9092	0.1811	0.052*
C6	1.2539 (4)	1.0555 (3)	−0.1110 (3)	0.0370 (5)
C7	1.3093 (5)	1.0269 (3)	−0.2441 (3)	0.0447 (6)
H7	1.2879	1.0908	−0.3082	0.054*
C3	1.1460 (6)	1.0973 (4)	0.1583 (4)	0.0549 (8)
H3	1.1094	1.1128	0.2476	0.066*
C8	1.3942 (5)	0.9057 (4)	−0.2799 (3)	0.0495 (7)
H8	1.4340	0.8876	−0.3686	0.059*
C9	1.4211 (4)	0.8100 (3)	−0.1843 (3)	0.0437 (6)
H9	1.4780	0.7269	−0.2086	0.052*
C5	1.1660 (5)	1.1797 (3)	−0.0655 (4)	0.0512 (8)
H5	1.1433	1.2478	−0.1255	0.061*
C4	1.1153 (6)	1.1986 (3)	0.0652 (4)	0.0607 (10)
H4	1.0590	1.2805	0.0940	0.073*
O10	0.6636 (2)	0.59823 (17)	0.58700 (16)	0.0282 (3)
O2	1.3962 (3)	0.65569 (19)	0.14615 (19)	0.0358 (4)
O3	1.3081 (3)	0.5195 (2)	−0.0816 (2)	0.0412 (4)
O4	0.2153 (3)	0.9054 (2)	0.4559 (3)	0.0549 (6)
H11	0.369 (4)	0.735 (3)	0.436 (3)	0.044 (10)*
H21	0.436 (5)	0.674 (4)	0.320 (2)	0.052 (11)*

H12	1.496 (3)	0.610 (3)	0.118 (4)	0.052 (11)*
H22	1.299 (3)	0.613 (3)	0.163 (4)	0.046 (10)*
H13	1.208 (4)	0.513 (4)	−0.013 (2)	0.052 (11)*
H23	1.264 (5)	0.505 (4)	−0.145 (2)	0.056 (11)*
H14	0.231 (5)	0.990 (2)	0.451 (4)	0.056 (11)*
H24	0.098 (3)	0.897 (3)	0.465 (4)	0.056 (11)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01923 (17)	0.02359 (18)	0.02047 (18)	0.00158 (13)	−0.00587 (13)	−0.00424 (13)
P2	0.0235 (2)	0.0164 (2)	0.0224 (2)	0.00486 (16)	−0.00927 (18)	−0.00462 (16)
P1	0.0217 (2)	0.0241 (2)	0.0155 (2)	0.00357 (17)	−0.00460 (16)	−0.00431 (17)
O5	0.0228 (7)	0.0389 (9)	0.0272 (8)	0.0059 (6)	−0.0095 (6)	−0.0111 (6)
O9	0.0451 (10)	0.0176 (7)	0.0457 (11)	0.0086 (6)	−0.0190 (8)	−0.0054 (7)
O8	0.0385 (9)	0.0262 (7)	0.0439 (10)	0.0039 (6)	−0.0270 (8)	−0.0061 (7)
O7	0.0277 (7)	0.0257 (7)	0.0277 (8)	−0.0016 (6)	−0.0009 (6)	−0.0091 (6)
O1	0.0473 (10)	0.0289 (8)	0.0294 (9)	0.0092 (7)	−0.0153 (8)	−0.0057 (7)
O6	0.0442 (10)	0.0516 (11)	0.0189 (7)	−0.0067 (9)	0.0032 (7)	−0.0060 (7)
C1	0.0319 (10)	0.0283 (10)	0.0328 (12)	0.0007 (8)	−0.0094 (9)	−0.0019 (8)
N1	0.0377 (11)	0.0283 (9)	0.0329 (11)	0.0020 (8)	−0.0050 (8)	0.0013 (8)
C2	0.0487 (15)	0.0478 (15)	0.0337 (13)	0.0005 (12)	−0.0135 (11)	−0.0072 (11)
C6	0.0421 (13)	0.0286 (11)	0.0394 (13)	−0.0012 (9)	−0.0137 (11)	0.0025 (9)
C7	0.0512 (16)	0.0462 (15)	0.0356 (14)	−0.0076 (12)	−0.0154 (12)	0.0092 (12)
C3	0.064 (2)	0.0542 (19)	0.0495 (18)	−0.0019 (16)	−0.0158 (16)	−0.0233 (15)
C8	0.0562 (18)	0.0559 (18)	0.0300 (13)	−0.0067 (14)	−0.0044 (12)	−0.0033 (12)
C9	0.0460 (15)	0.0368 (13)	0.0383 (14)	0.0024 (11)	0.0004 (11)	−0.0071 (11)
C5	0.0574 (19)	0.0280 (12)	0.069 (2)	0.0018 (12)	−0.0237 (16)	−0.0006 (13)
C4	0.062 (2)	0.0364 (15)	0.082 (3)	0.0054 (14)	−0.0164 (19)	−0.0267 (17)
O10	0.0251 (7)	0.0347 (8)	0.0249 (7)	−0.0022 (6)	−0.0056 (6)	−0.0095 (6)
O2	0.0398 (10)	0.0339 (9)	0.0312 (9)	0.0008 (7)	−0.0094 (8)	0.0001 (7)
O3	0.0451 (11)	0.0543 (12)	0.0253 (9)	0.0030 (9)	−0.0129 (8)	−0.0072 (8)
O4	0.0449 (12)	0.0263 (9)	0.091 (2)	0.0085 (8)	−0.0178 (12)	−0.0164 (11)

Geometric parameters (Å, º)

Co1—O10^{i}	2.1064 (16)	N1—H1	0.8600
Co1—O10	2.1064 (16)	C2—C3	1.361 (5)
Co1—O1^{i}	2.1127 (18)	C2—H2	0.9300
Co1—O1	2.1127 (18)	C6—C7	1.402 (4)
Co1—O5^{i}	2.1159 (16)	C6—C5	1.421 (4)
Co1—O5	2.1159 (16)	C7—C8	1.362 (5)
P2—O9	1.4737 (17)	C7—H7	0.9300
P2—O10	1.4748 (17)	C3—C4	1.403 (6)
P2—O8	1.5963 (17)	C3—H3	0.9300
P2—O7	1.6029 (16)	C8—C9	1.377 (5)
P1—O6	1.4730 (18)	C8—H8	0.9300
P1—O5	1.4779 (17)	C9—H9	0.9300

P1—O8^{ii}	1.5833 (18)	C5—C4	1.354 (6)
P1—O7	1.5913 (17)	C5—H5	0.9300
O8—P1^{ii}	1.5833 (18)	C4—H4	0.9300
O1—H11	0.830 (17)	O2—H12	0.827 (17)
O1—H21	0.831 (17)	O2—H22	0.825 (17)
C1—N1	1.372 (3)	O3—H13	0.863 (17)
C1—C6	1.401 (4)	O3—H23	0.875 (17)
C1—C2	1.402 (4)	O4—H14	0.855 (18)
N1—C9	1.326 (4)	O4—H24	0.855 (17)

O10^{i}—Co1—O10	180.00 (8)	N1—C1—C2	119.6 (2)
O10^{i}—Co1—O1^{i}	90.99 (7)	C6—C1—C2	122.1 (3)
O10—Co1—O1^{i}	89.01 (7)	C9—N1—C1	122.4 (2)
O10^{i}—Co1—O1	89.01 (7)	C9—N1—H1	118.8
O10—Co1—O1	90.99 (7)	C1—N1—H1	118.8
O1^{i}—Co1—O1	180.0	C3—C2—C1	118.3 (3)
O10^{i}—Co1—O5^{i}	89.95 (6)	C3—C2—H2	120.8
O10—Co1—O5^{i}	90.05 (6)	C1—C2—H2	120.8
O1^{i}—Co1—O5^{i}	86.22 (7)	C1—C6—C7	118.8 (3)
O1—Co1—O5^{i}	93.78 (7)	C1—C6—C5	117.5 (3)
O10^{i}—Co1—O5	90.05 (6)	C7—C6—C5	123.7 (3)
O10—Co1—O5	89.95 (6)	C8—C7—C6	120.1 (3)
O1^{i}—Co1—O5	93.78 (7)	C8—C7—H7	119.9
O1—Co1—O5	86.22 (7)	C6—C7—H7	119.9
O5^{i}—Co1—O5	180.0	C2—C3—C4	120.8 (3)
O9—P2—O10	121.11 (11)	C2—C3—H3	119.6
O9—P2—O8	105.29 (10)	C4—C3—H3	119.6
O10—P2—O8	110.13 (10)	C7—C8—C9	119.8 (3)
O9—P2—O7	108.09 (10)	C7—C8—H8	120.1
O10—P2—O7	109.91 (9)	C9—C8—H8	120.1
O8—P2—O7	100.23 (10)	N1—C9—C8	120.5 (3)
O6—P1—O5	117.41 (11)	N1—C9—H9	119.7
O6—P1—O8^{ii}	109.43 (12)	C8—C9—H9	119.7
O5—P1—O8^{ii}	106.81 (10)	C4—C5—C6	119.9 (3)
O6—P1—O7	106.60 (11)	C4—C5—H5	120.0
O5—P1—O7	111.38 (9)	C6—C5—H5	120.0
O8^{ii}—P1—O7	104.47 (10)	C5—C4—C3	121.3 (3)
P1—O5—Co1	130.02 (10)	C5—C4—H4	119.3
P1^{ii}—O8—P2	137.26 (12)	C3—C4—H4	119.3
P1—O7—P2	134.40 (11)	P2—O10—Co1	131.90 (10)
Co1—O1—H11	117 (2)	H12—O2—H22	113 (3)
Co1—O1—H21	116 (3)	H13—O3—H23	102 (2)
H11—O1—H21	110 (2)	H14—O4—H24	107 (3)
N1—C1—C6	118.3 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.86	1.88	2.728 (3)	171
O1—H11···O4	0.83 (3)	1.98 (3)	2.747 (3)	154 (3)
O1—H21···O2^{iii}	0.84 (3)	2.00 (3)	2.841 (3)	179 (4)
O2—H12···O3^{iv}	0.83 (3)	1.85 (3)	2.666 (3)	168 (3)
O2—H22···O6	0.83 (3)	1.95 (3)	2.771 (3)	172 (4)
O3—H13···O6	0.86 (2)	1.95 (2)	2.743 (3)	152 (3)
O3—H23···O5^{v}	0.87 (3)	2.02 (2)	2.833 (3)	154 (3)
O4—H14···O9^{vi}	0.86 (2)	2.01 (2)	2.824 (3)	157 (4)
O4—H24···O9^{iii}	0.86 (3)	2.06 (3)	2.890 (3)	163 (3)
C7—H7···O9^{vii}	0.93	2.59	3.459 (4)	156
C9—H9···O3	0.93	2.54	3.080 (4)	118
C9—H9···O10^{viii}	0.93	2.59	3.381 (3)	143

Symmetry codes: (iii) $x-1, y, z$; (iv) $-x+3, -y+1, -z$; (v) $-x+2, -y+1, -z$; (vi) $-x+1, -y+2, -z+1$; (vii) $-x+2, -y+2, -z$; (viii) $x+1, y, z-1$.