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catena-Poly[[[aquaformato(1,10-phenanthroline)cobalt(II)]-μ-formato] monohydrate]

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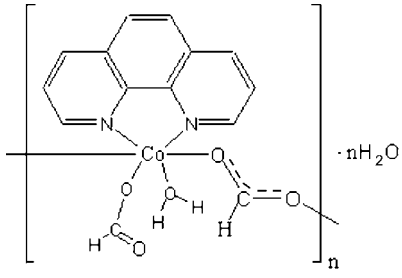
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.007 Å; R factor = 0.043; wR factor = 0.100; data-to-parameter ratio = 12.3.

In the polymeric title compound, $\{[Co(CHO_2)_2(C_{12}H_8N_2)(H_2O)]\cdot H_2O\}_n$, the cobalt ion is coordinated by two N atoms from one chelating 1,10-phenanthroline ligand, three formate O atoms and one water O atom, giving a *cis*-CoN_2O_4 octahedral geometry. Pairs of formate anions bridge the metal atoms into a chain. A network of O—H···O hydrogen bonds helps to establish the packing.

Related literature

For background, see: Peng *et al.* (2006); Cui *et al.* (2007).



Experimental

Crystal data

$[Co(CHO_2)_2(C_{12}H_8N_2)(H_2O)]\cdot H_2O$
M_r = 365.20
Orthorhombic, $Pna2_1$
a = 18.908 (4) Å
b = 12.014 (2) Å
c = 6.3685 (13) Å
V = 1446.7 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.22 mm^{-1}
T = 113 (2) K
0.20 × 0.18 × 0.08 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.792, T_{max} = 0.909
8676 measured reflections
2562 independent reflections
2153 reflections with $I > 2\sigma(I)$
R_{int} = 0.085

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.100
S = 0.86
2562 reflections
209 parameters
7 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}
Absolute structure: Flack (1983), 1152 Friedel pairs
Flack parameter: 0.00 (3)

Table 1
Selected bond lengths (Å).

Co1—O1	2.060 (3)	Co1—N1	2.107 (4)
Co1—O5	2.082 (3)	Co1—O3	2.129 (3)
Co1—O4^{i}	2.086 (3)	Co1—N2	2.146 (4)

Symmetry code: (i) $-x+1, -y+1, z-\frac{1}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O6^{ii}	0.85	1.83	2.644 (4)	159
O6—H6A···O2^{iii}	0.85	1.93	2.734 (4)	156
O5—H5B···O4	0.85	1.82	2.653 (4)	167
O6—H6B···O2	0.85	1.90	2.755 (5)	178

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2527).

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supplementary materials

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catena-Poly[[[aquaformato(1,10-phenanthroline)cobalt(II)]-μ-formato] monohydrate]

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Comment

Recently, formate complexes have received attention in terms of their structure, magnetism and biological activity (Peng *et al.*, 2006; Cui *et al.*, 2007).

We report here the structure (Fig. 1) of the polymeric title compound, (I), in which two formate anions are bridging between Co centres. The cobalt coordinaion is completed by a monodentate-O terminal formate ion, an N,*N*-bidentate 1,10-phenanthroline molecule and a water molecule. This results in a distorted *cis*-CoN_2O_4 octahedral coordination gemoetry (Table 1).

The bridging formate anions lead to a one-dimensional polymeric chain. The packing for (I) is consolidated by a network of O—H···O hydrogen bonds (Table 2).

Experimental

The title compound was prepared by adding 5 ml of aqueous solution of cobalt nitrate (0.146 g, 0.5 mmol), to 10 ml of ethanol solution of 1,10-phenanthroline (0.099 g, 0.5 mmol), after which sodium formate (0.232 g, 4 mmol) was added and was refluexed for 2 h. The resulting solution was filtrated and the filtrate was kept at room temperature and orange blocks of (I) appeared after a week.

Refinement

The H atoms were positioned geometrically (C—H = 0.96–0.97 Å, O—H = 0.85 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier).

Figures

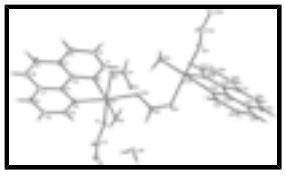


Fig. 1. A view of a fragemnt of the polymeric structure of (I). Displacement ellopsoids are drawn at the 30% probability level and H atoms are shown as spheres of arbitrary radius. Atoms with a suffix A are at the symmetry position (1 − *x*, 1 − *y*, *z* − 1/2).

catena-Poly[[[aquaformato(1,10-phenanthroline)cobalt(II)]-μ-formato] monohydrate]

Crystal data

$[Co(CHO_2)_2(C_{12}H_8N_2)(H_2O)]\cdot H_2O$	D_x = 1.677 Mg m^{-3}
M_r = 365.20	Mo *K*α radiation

	λ = 0.71073 Å
Orthorhombic, $Pna2_1$	Cell parameters from 3127 reflections
a = 18.908 (4) Å	θ = 2.0–27.9º
b = 12.014 (2) Å	μ = 1.22 mm^{-1}
c = 6.3685 (13) Å	T = 113 (2) K
V = 1446.7 (5) $Å^3$	Block, orange
Z = 4	0.20 × 0.18 × 0.08 mm
F_{000} = 748	

Data collection

Rigaku Saturn diffractometer	2562 independent reflections
Radiation source: rotating anode	2153 reflections with $I > 2\sigma(I)$
Monochromator: confocal	R_{int} = 0.085
T = 113(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 2.7º
Absorption correction: multi-scan (CrystalClear; Rigaku/MSC, 2005)	h = −22→22
T_{min} = 0.792, T_{max} = 0.909	k = −11→14
8676 measured reflections	l = −7→7

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.043	$w = 1/[\sigma^2(F_o^2) + (0.0651P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.100	$(\Delta/\sigma)_{max}$ = 0.001
S = 0.86	$\Delta\rho_{max}$ = 0.33 e $Å^{-3}$
2562 reflections	$\Delta\rho_{min}$ = −0.42 e $Å^{-3}$
209 parameters	Extinction correction: none
7 restraints	Absolute structure: Flack (1983), 1152 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.00 (3)
Secondary atom site location: difference Fourier map	

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.58489 (2)	0.37977 (4)	0.81148 (10)	0.01363 (16)
O1	0.57437 (16)	0.2373 (2)	0.6343 (5)	0.0212 (8)
O2	0.56006 (18)	0.0562 (2)	0.5806 (6)	0.0273 (8)
O3	0.59367 (14)	0.5412 (2)	0.9471 (5)	0.0177 (7)
O4	0.49223 (15)	0.5437 (2)	1.1272 (5)	0.0186 (7)
O5	0.50825 (16)	0.3308 (2)	1.0273 (5)	0.0209 (8)
H5A	0.5086	0.2784	1.1163	0.025*
H5B	0.4983	0.3956	1.0733	0.025*
N1	0.66885 (18)	0.4293 (3)	0.6150 (6)	0.0136 (8)
N2	0.67416 (19)	0.3116 (3)	0.9751 (6)	0.0173 (8)
C1	0.6659 (3)	0.4838 (4)	0.4355 (7)	0.0208 (10)
H1	0.6218	0.5067	0.3880	0.025*
C2	0.7245 (2)	0.5094 (3)	0.3127 (10)	0.0240 (9)
H2	0.7193	0.5481	0.1871	0.029*
C3	0.7901 (2)	0.4762 (4)	0.3807 (8)	0.0253 (12)
H3	0.8301	0.4913	0.3007	0.030*
C4	0.7962 (2)	0.4191 (4)	0.5731 (8)	0.0214 (11)
C5	0.8627 (3)	0.3794 (4)	0.6570 (9)	0.0323 (13)
H5	0.9045	0.3951	0.5862	0.039*
C6	0.8646 (2)	0.3205 (4)	0.8352 (10)	0.0319 (13)
H6	0.9080	0.2957	0.8852	0.038*
C7	0.8015 (2)	0.2944 (4)	0.9519 (8)	0.0235 (11)
C8	0.8010 (3)	0.2328 (4)	1.1383 (8)	0.0268 (12)
H8	0.8432	0.2066	1.1942	0.032*
C9	0.7387 (3)	0.2112 (4)	1.2382 (8)	0.0292 (13)
H9	0.7382	0.1696	1.3614	0.035*
C10	0.6751 (2)	0.2524 (3)	1.1525 (8)	0.0226 (11)
H10	0.6327	0.2380	1.2214	0.027*
C11	0.7362 (2)	0.3326 (4)	0.8765 (7)	0.0181 (10)
C12	0.7338 (2)	0.3958 (4)	0.6843 (8)	0.0183 (11)
C13	0.5675 (2)	0.1395 (4)	0.6949 (8)	0.0225 (11)
H13	0.5679	0.1275	0.8391	0.027*
C14	0.5454 (2)	0.5899 (4)	1.0437 (7)	0.0169 (10)
H14	0.5488	0.6669	1.0554	0.020*
O6	0.49393 (19)	0.1397 (2)	0.2288 (6)	0.0332 (9)
H6A	0.4752	0.0902	0.1500	0.040*
H6B	0.5149	0.1157	0.3384	0.040*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0135 (3)	0.0126 (3)	0.0147 (3)	0.0009 (2)	−0.0011 (3)	0.0004 (3)

O1	0.0298 (19)	0.0150 (18)	0.0187 (19)	0.0002 (13)	−0.0043 (14)	0.0023 (15)
O2	0.044 (2)	0.0148 (17)	0.0235 (18)	−0.0011 (15)	−0.0075 (16)	−0.0029 (16)
O3	0.0163 (16)	0.0160 (17)	0.0207 (18)	0.0009 (12)	0.0034 (13)	0.0012 (15)
O4	0.0172 (16)	0.0181 (16)	0.0203 (18)	−0.0024 (13)	0.0056 (14)	0.0011 (14)
O5	0.0251 (17)	0.0109 (16)	0.027 (2)	0.0023 (12)	0.0103 (15)	0.0023 (14)
N1	0.016 (2)	0.0094 (18)	0.016 (2)	0.0001 (14)	−0.0008 (16)	−0.0020 (17)
N2	0.018 (2)	0.0143 (19)	0.020 (2)	0.0029 (15)	−0.0013 (16)	−0.0040 (18)
C1	0.029 (3)	0.018 (2)	0.016 (2)	0.0018 (19)	0.002 (2)	−0.002 (2)
C2	0.035 (2)	0.017 (2)	0.020 (2)	−0.0100 (17)	0.005 (3)	−0.003 (3)
C3	0.029 (3)	0.017 (3)	0.030 (3)	−0.008 (2)	0.014 (2)	−0.011 (2)
C4	0.019 (3)	0.018 (2)	0.027 (3)	−0.0049 (18)	0.006 (2)	−0.008 (2)
C5	0.011 (3)	0.046 (3)	0.041 (3)	−0.002 (2)	0.005 (2)	−0.020 (3)
C6	0.018 (2)	0.038 (3)	0.039 (4)	0.0110 (19)	−0.012 (3)	−0.021 (3)
C7	0.022 (3)	0.023 (3)	0.026 (3)	0.005 (2)	−0.007 (2)	−0.009 (2)
C8	0.032 (3)	0.019 (3)	0.030 (3)	0.009 (2)	−0.014 (2)	−0.011 (2)
C9	0.039 (3)	0.030 (3)	0.019 (2)	0.005 (2)	−0.014 (2)	−0.006 (2)
C10	0.032 (3)	0.012 (2)	0.024 (3)	0.0009 (19)	−0.006 (2)	0.000 (2)
C11	0.021 (2)	0.014 (2)	0.019 (3)	0.0056 (18)	−0.0033 (18)	−0.0070 (19)
C12	0.016 (2)	0.016 (2)	0.023 (3)	0.0020 (18)	0.000 (2)	−0.009 (2)
C13	0.022 (3)	0.025 (3)	0.020 (3)	0.005 (2)	0.002 (2)	0.000 (2)
C14	0.015 (2)	0.015 (2)	0.021 (3)	0.0028 (18)	−0.0028 (19)	−0.001 (2)
O6	0.052 (2)	0.0204 (18)	0.027 (2)	−0.0118 (15)	−0.0135 (17)	0.0055 (16)

Geometric parameters (Å, °)

Co1—O1	2.060 (3)	C3—C4	1.409 (7)
Co1—O5	2.082 (3)	C3—H3	0.9300
Co1—O4^{i}	2.086 (3)	C4—C12	1.404 (6)
Co1—N1	2.107 (4)	C4—C5	1.446 (7)
Co1—O3	2.129 (3)	C5—C6	1.338 (8)
Co1—N2	2.146 (4)	C5—H5	0.9300
O1—C13	1.244 (5)	C6—C7	1.440 (7)
O2—C13	1.245 (5)	C6—H6	0.9300
O3—C14	1.246 (5)	C7—C8	1.398 (7)
O4—C14	1.266 (5)	C7—C11	1.402 (6)
O4—Co1^{ii}	2.086 (3)	C8—C9	1.363 (7)
O5—H5A	0.8473	C8—H8	0.9300
O5—H5B	0.8533	C9—C10	1.411 (6)
N1—C1	1.319 (6)	C9—H9	0.9300
N1—C12	1.366 (6)	C10—H10	0.9300
N2—C10	1.335 (6)	C11—C12	1.441 (7)
N2—C11	1.355 (6)	C13—H13	0.9300
C1—C2	1.389 (6)	C14—H14	0.9300
C1—H1	0.9300	O6—H6A	0.8544
C2—C3	1.375 (6)	O6—H6B	0.8532
C2—H2	0.9300		
O1—Co1—O5	93.42 (12)	C4—C3—H3	120.4
O1—Co1—O4^{i}	89.45 (11)	C12—C4—C3	117.9 (4)

O5—Co1—O4^{i}	90.54 (12)	C12—C4—C5	118.5 (5)
O1—Co1—N1	88.97 (13)	C3—C4—C5	123.5 (4)
O5—Co1—N1	174.97 (14)	C6—C5—C4	120.7 (5)
O4^{i}—Co1—N1	93.91 (13)	C6—C5—H5	119.6
O1—Co1—O3	170.57 (13)	C4—C5—H5	119.6
O5—Co1—O3	92.52 (12)	C5—C6—C7	122.1 (4)
O4^{i}—Co1—O3	83.18 (11)	C5—C6—H6	119.0
N1—Co1—O3	85.70 (12)	C7—C6—H6	119.0
O1—Co1—N2	91.42 (13)	C8—C7—C11	117.2 (4)
O5—Co1—N2	96.83 (14)	C8—C7—C6	124.0 (4)
O4^{i}—Co1—N2	172.51 (14)	C11—C7—C6	118.7 (5)
N1—Co1—N2	78.67 (13)	C9—C8—C7	120.2 (4)
O3—Co1—N2	95.14 (13)	C9—C8—H8	119.9
C13—O1—Co1	128.7 (3)	C7—C8—H8	119.9
C14—O3—Co1	124.8 (3)	C8—C9—C10	119.3 (5)
C14—O4—Co1^{ii}	126.8 (3)	C8—C9—H9	120.4
Co1—O5—H5A	130.2	C10—C9—H9	120.4
Co1—O5—H5B	97.0	N2—C10—C9	121.7 (5)
H5A—O5—H5B	116.8	N2—C10—H10	119.1
C1—N1—C12	117.6 (4)	C9—C10—H10	119.1
C1—N1—Co1	128.6 (3)	N2—C11—C7	122.9 (4)
C12—N1—Co1	113.7 (3)	N2—C11—C12	117.7 (4)
C10—N2—C11	118.7 (4)	C7—C11—C12	119.4 (4)
C10—N2—Co1	128.7 (3)	N1—C12—C4	122.3 (5)
C11—N2—Co1	112.7 (3)	N1—C12—C11	117.2 (4)
N1—C1—C2	124.4 (5)	C4—C12—C11	120.5 (4)
N1—C1—H1	117.8	O1—C13—O2	126.1 (5)
C2—C1—H1	117.8	O1—C13—H13	116.9
C3—C2—C1	118.5 (5)	O2—C13—H13	116.9
C3—C2—H2	120.7	O3—C14—O4	125.7 (4)
C1—C2—H2	120.7	O3—C14—H14	117.2
C2—C3—C4	119.3 (5)	O4—C14—H14	117.2
C2—C3—H3	120.4	H6A—O6—H6B	116.0
O5—Co1—O1—C13	−41.7 (4)	C4—C5—C6—C7	−0.3 (7)
O4^{i}—Co1—O1—C13	−132.2 (4)	C5—C6—C7—C8	179.8 (5)
N1—Co1—O1—C13	133.9 (4)	C5—C6—C7—C11	−0.4 (7)
N2—Co1—O1—C13	55.3 (4)	C11—C7—C8—C9	0.6 (7)
O5—Co1—O3—C14	−27.5 (3)	C6—C7—C8—C9	−179.6 (4)
O4^{i}—Co1—O3—C14	62.8 (3)	C7—C8—C9—C10	−0.6 (7)
N1—Co1—O3—C14	157.2 (4)	C11—N2—C10—C9	−0.3 (6)
N2—Co1—O3—C14	−124.6 (3)	Co1—N2—C10—C9	178.6 (3)
O1—Co1—N1—C1	86.0 (4)	C8—C9—C10—N2	0.5 (7)
O4^{i}—Co1—N1—C1	−3.4 (4)	C10—N2—C11—C7	0.4 (6)
O3—Co1—N1—C1	−86.2 (4)	Co1—N2—C11—C7	−178.7 (3)
N2—Co1—N1—C1	177.6 (4)	C10—N2—C11—C12	179.5 (4)
O1—Co1—N1—C12	−91.7 (3)	Co1—N2—C11—C12	0.4 (5)
O4^{i}—Co1—N1—C12	179.0 (3)	C8—C7—C11—N2	−0.5 (7)

O3—Co1—N1—C12	96.1 (3)	C6—C7—C11—N2	179.7 (4)
N2—Co1—N1—C12	0.0 (3)	C8—C7—C11—C12	−179.6 (4)
O1—Co1—N2—C10	−90.5 (4)	C6—C7—C11—C12	0.6 (6)
O5—Co1—N2—C10	3.1 (4)	C1—N1—C12—C4	1.0 (6)
N1—Co1—N2—C10	−179.2 (4)	Co1—N1—C12—C4	178.9 (3)
O3—Co1—N2—C10	96.2 (4)	C1—N1—C12—C11	−177.7 (4)
O1—Co1—N2—C11	88.4 (3)	Co1—N1—C12—C11	0.2 (5)
O5—Co1—N2—C11	−178.0 (3)	C3—C4—C12—N1	−1.9 (6)
N1—Co1—N2—C11	−0.2 (3)	C5—C4—C12—N1	−179.4 (4)
O3—Co1—N2—C11	−84.8 (3)	C3—C4—C12—C11	176.8 (4)
C12—N1—C1—C2	0.0 (6)	C5—C4—C12—C11	−0.7 (6)
Co1—N1—C1—C2	−177.6 (3)	N2—C11—C12—N1	−0.4 (6)
N1—C1—C2—C3	0.0 (7)	C7—C11—C12—N1	178.7 (4)
C1—C2—C3—C4	−0.9 (7)	N2—C11—C12—C4	−179.2 (4)
C2—C3—C4—C12	1.8 (6)	C7—C11—C12—C4	0.0 (7)
C2—C3—C4—C5	179.2 (4)	Co1—O1—C13—O2	178.7 (3)
C12—C4—C5—C6	0.9 (7)	Co1—O3—C14—O4	20.8 (6)
C3—C4—C5—C6	−176.4 (5)	Co1^{ii}—O4—C14—O3	174.4 (3)

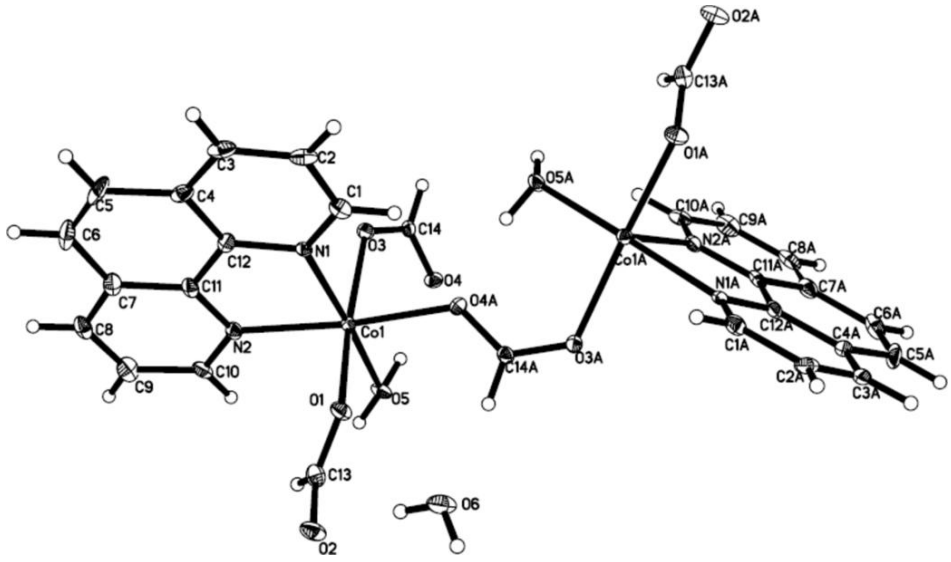
Symmetry codes: (i) −*x*+1, −*y*+1, *z*−1/2; (ii) −*x*+1, −*y*+1, *z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5A···O6^{iii}	0.85	1.83	2.644 (4)	159
O6—H6A···O2^{iv}	0.85	1.93	2.734 (4)	156
O5—H5B···O4	0.85	1.82	2.653 (4)	167
O6—H6B···O2	0.85	1.90	2.755 (5)	178

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

Fig. 1


O2A
C13A
O1A
O5A
C10A
C9A
N2A
C8A
C11A
C7A
N1A
C12A
C6A
C4A
C5A
C1A
C2A
C3A
Co1A
O3A
C14A
O4A
C3
C2
C1
C4
C5
C6
C12
N1
O3
C14
O4
C11
C7
C8
N2
Co1
C10
C9
O1
O5
C13
O2
O6