



Synthesis, crystal structure and Hirshfeld surface analysis of tetraaquabis(isonicotinamide- κN^1)-cobalt(II) succinate

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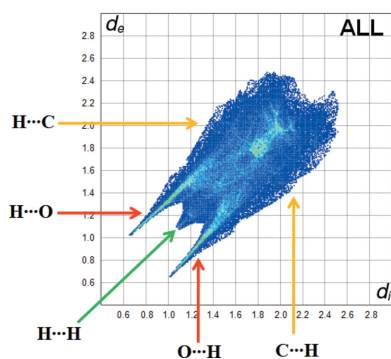
The reaction of CoCl_2 with succinic acid and isonicotinamide in basic solution produces the title complex $[\text{Co}(\text{C}_6\text{H}_6\text{N}_2\text{O})_2(\text{H}_2\text{O})_4](\text{C}_4\text{H}_4\text{O}_4)$. The cobalt(II) ion of the complex cation and the succinate anion are each located on an inversion centre. The Co^{II} ion is octahedrally coordinated by four O atoms of water molecules and two N atoms of isonicotinamide molecules. The two ions are linked *via* $\text{O}_{\text{water}}-\text{H}\cdots\text{O}_{\text{succinate}}$ hydrogen bonds, forming chains propagating along [001]. In the crystal, these hydrogen-bonded chains are linked into a three-dimensional framework by further $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds and $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds. The framework is reinforced by $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds. Hirshfeld surface analysis and two-dimensional fingerprint plots have been used to analyse the intermolecular interactions present in the crystal.

1. Chemical context

Metal carboxylates have attracted intense attention because of their interesting framework topologies. Among metal carboxylates, succinate dianions (succ) have good conformational freedom and they possess some desirable features such as being a versatile ligand because of the four electron-donor oxygen atoms they carry, and their ability to link inorganic moieties. Metal succinates are one of the best dicarboxylate-based moieties that display an interesting structural variety. Dicarboxylic acids such as succinic acid and amides have been particularly useful in creating many supramolecular structures between isonicotinamide and a variety of carboxylic acid molecules (Vishweshwar *et al.*, 2003; Aakeröy *et al.*, 2002). Dicarboxylic acid ligands have been utilized frequently in the synthesis of various metal carboxylates. For this reason they have been investigated widely, both experimentally and computationally. We describe herein the synthesis, structural features and Hirshfeld surface analysis of a new tetraaquabis(isonicotinamide- κN^1)cobalt(II) succinate complex.

2. Structural commentary

The molecular structure of the title complex is illustrated in Fig. 1. The cobalt(II) ion is coordinated octahedrally by four O atoms of water molecules and two $\text{N}_{\text{pyridine}}$ atoms of isonicotinamide molecules. The values of the $\text{Co}-\text{O}_{\text{water}}$ and $\text{Co}-\text{N}_{\text{pyridine}}$ bond lengths and the bond angles involving atom Co1 (Table 1) are close to those reported for similar cobalt(II) complexes (Gao *et al.*, 2006; Liu *et al.*, 2012). The C—O bond



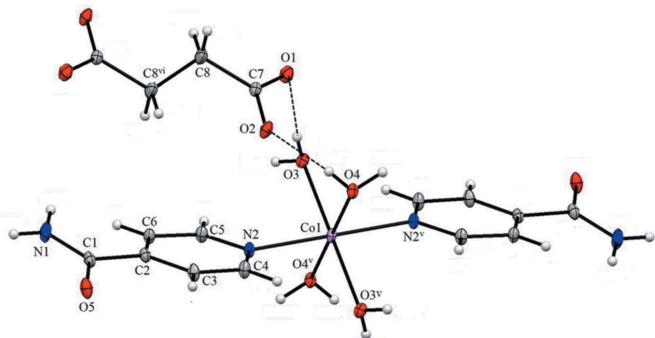
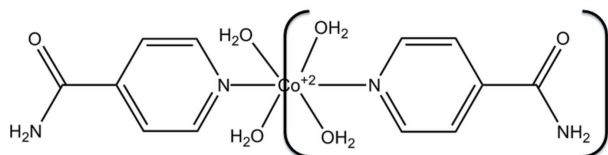
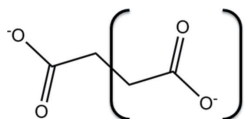


Figure 1
The molecular structure of the title complex, with the atom labelling. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (v) $-x + 1, -y + 1, -z + 2$; (vi) $-x + 1, -y + 1, -z + 1$.]

lengths in the deprotonated carboxylic groups of the succinate dianion are almost the same, *viz.* 1.247 (3) Å for C7—O1 and 1.257 (3) Å for C7—O2, indicating delocalization of charge. Each O atom of the succinate dianion is linked to an H atom of a water molecule *via* O—H···O hydrogen bonds, so forming chains along the *c*-axis direction (Table 2 and Figs. 1 and 2).



3. Supramolecular features

In the crystal, the chains formed by O—H···O hydrogen bonds involving the succinate anions and the complex cations are linked by further O—H···O and N—H···O hydrogen

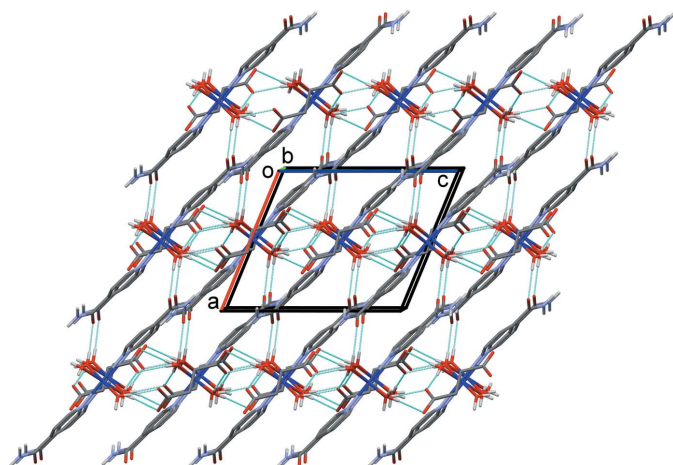


Figure 2
A view along the *b* axis of the crystal packing of the title complex. Dashed lines indicate the hydrogen bonds (see Table 2).

Table 1
Selected geometric parameters (Å, °).

Co1—O3	2.1134 (15)	Co1—N2	2.1540 (16)
Co1—O4	2.0795 (16)		
O4—Co1—N2 ⁱ	92.15 (7)	O3—Co1—N2 ⁱ	88.85 (6)
O4—Co1—N2	87.85 (6)	O4 ⁱ —Co1—O3	88.82 (7)
O3—Co1—N2	91.15 (6)	O4—Co1—O3	91.18 (7)

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

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

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O3—H3B···O1	0.79 (4)	1.97 (4)	2.756 (3)	176 (3)
O4—H4A···O2	0.77 (3)	1.88 (3)	2.651 (2)	174 (3)
O3—H3A···O2 ⁱⁱ	0.81 (3)	1.92 (3)	2.729 (2)	175 (3)
O4—H4B···O5 ⁱⁱⁱ	0.83 (4)	1.97 (4)	2.801 (2)	174 (3)
N1—H1A···O5 ^{iv}	0.92 (4)	2.34 (4)	3.227 (3)	160 (3)
N1—H1B···O1 ^v	0.87 (4)	2.14 (4)	2.966 (3)	160 (3)
C5—H5···O2 ⁱⁱ	0.93	2.41	3.307 (3)	161
C6—H6···O5 ^{iv}	0.93	2.31	3.223 (3)	167

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

bonds, forming a three-dimensional supramolecular architecture (Table 2 and Fig. 2). Within the framework, C—H···O hydrogen bonds are also present (Table 2).

4. Hirshfeld surface analysis

CrystalExplorer17.5 (Turner *et al.*, 2017) was used to analyse the interactions in the crystal. The molecular Hirshfeld surfaces were obtained using a standard (high) surface resolution with the three-dimensional d_{norm} surfaces mapped over a fixed colour scale of -0.728 (red) to 1.428 (blue). The red spots in the d_{norm} surface (Fig. 3), indicate the regions of donor–acceptor interactions given in Table 2.

The view of the three-dimensional Hirshfeld surface of the title compound plotted over electrostatic potential energy in the range -0.366 to 0.236 a.u. using the STO-3G basis set at the Hartree–Fock level of theory is given in Fig. 4. The C—H···O, N—H···O and O—H···O hydrogen-bond donors and acceptors are shown as blue and red areas around the related

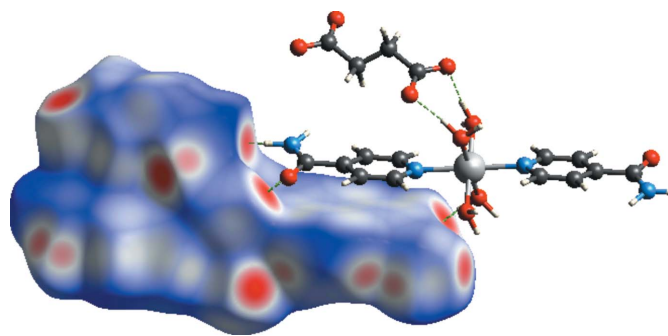


Figure 3
 d_{norm} mapped on the Hirshfeld surfaces to visualize the intramolecular and intermolecular interactions of the title complex.

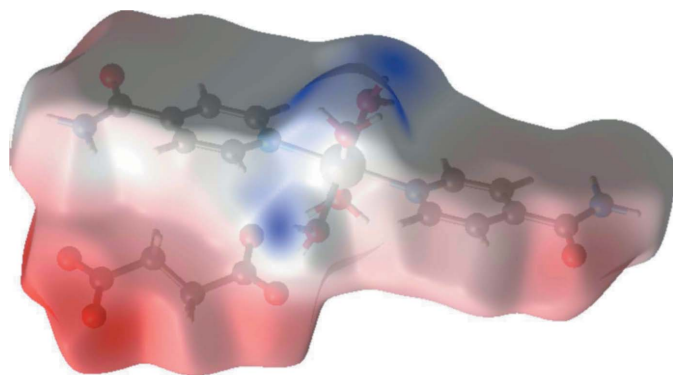


Figure 4
A view of the three-dimensional Hirshfeld surface of the title complex, plotted over the electrostatic potential energy.

atoms with positive (hydrogen-bond donors) and negative (hydrogen-bond acceptors) electrostatic potentials, respectively.

The fingerprint plot for the title complex is presented in Fig. 5. The contribution from the O \cdots H/H \cdots O contacts, corresponding to C–H \cdots O, N–H \cdots O and O–H \cdots O interactions, is represented by a pair of sharp spikes characteristic of a strong hydrogen-bonding interaction (43%) (Fig. 6a). The H \cdots H interactions appear in the middle of the scattered points in the two-dimensional fingerprint plots with an overall Hirshfeld surface of 39.8% (Fig. 6b). The contribution of the other intermolecular contacts to the Hirshfeld surfaces is C \cdots H/H \cdots C (8.4%) (Fig. 6c). The C \cdots C/C \cdots C contacts with 3.8% contribution appear as points of low density (Fig. 6d).

5. Database survey

A search of the Cambridge Structural Database (CSD, version 5.39, update May 2018; Groom *et al.*, 2016) revealed the structures of five similar tetraaquabis(isonicotinamide-

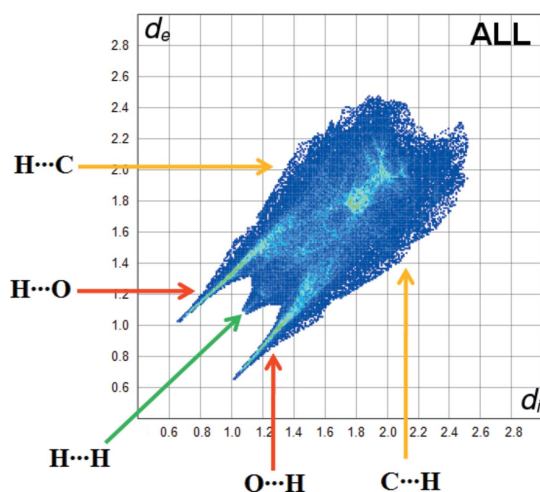


Figure 5
The fingerprint plot of the title compound.

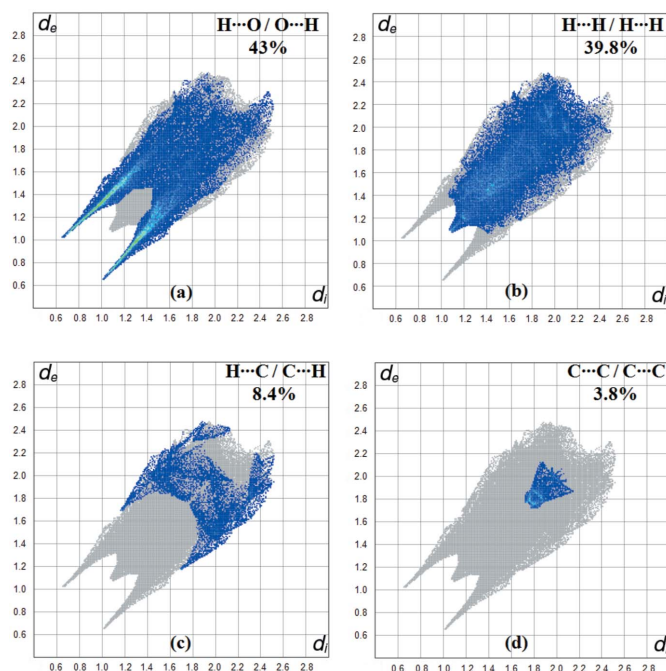


Figure 6
(a) H \cdots O/O \cdots H, (b) H \cdots H/H \cdots H, (c) H \cdots C/C \cdots H and (d) C \cdots C/C \cdots C contacts in the title complex, showing the percentages of contacts contributing to the total Hirshfeld surface area.

κN^1)cobalt(II) complexes with different counter-anions. They include *p*-formylbenzoate dihydrate (HUCPIF; Hökelek *et al.*, 2009), bis(3-hydroxybenzoate) tetrahydrate (LAMMOD; Zaman *et al.*, 2012), disaccharinate sesquihydrate (LEHHUC; Uçar *et al.*, 2006), bis(thiophene-2,5-dicarboxylate) dihydrate (NETQOU; Liu *et al.*, 2012) and terephthalate dihydrate (SETHIJ; Gao *et al.*, 2006). In all five complexes the cation possesses inversion symmetry with the cobalt ion being located on a centre of symmetry. The Co–O_{water} bond lengths vary from *ca* 2.057 to 2.115 Å, while the Co–N_{pyridine} bond lengths vary from *ca* 2.131 to 2.169 Å. In the title complex, the cation also possesses inversion symmetry and the Co–O_{water} bond lengths [2.079 (2) and 2.113 (2) Å] and the Co–N_{pyridine} bond length [2.154 (2) Å] fall within these limits. In addition, there are several precedents for succinic acid and isonicotinamides, including the structures of bis(isonicotinamide) succinic acid (Aakeröy *et al.*, 2002), succinic acid *N,N'*-octane-1,8-diyl-diisonicotinamide (Aakeröy *et al.*, 2014), succinic acid bis(isonicotinamide) (Vishweshwar *et al.*, 2003) and *catena*-[(μ_4 -succinato)(μ_2 -succinato)bis(μ_2 -4-pyridylisonicotinamide)dizinc] (Uebler *et al.*, 2013).

6. Synthesis and crystallization

An aqueous solution of succinic acid (25 mmol, 3 g) was added to a solution of NaOH (50 mmol, 2 g) under stirring. An aqueous solution of CoCl₂·6H₂O (25 mmol, 5.95 g) was added and the reaction mixture stirred for 30 min at room temperature. The pink mixture obtained was filtered and left to dry. The pink crystalline material (0.86 mmol, 0.20 g)

Table 3
Experimental details.

Crystal data	
Chemical formula	[Co(C ₆ H ₆ N ₂ O) ₂ (H ₂ O) ₄](C ₄ H ₄ O ₄)
<i>M_r</i>	491.32
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.6757 (8), 10.0381 (8), 11.4947 (10)
β (°)	112.489 (6)
<i>V</i> (Å ³)	1031.53 (15)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.89
Crystal size (mm)	0.68 × 0.49 × 0.37
Data collection	
Diffraction	Stoe <i>IPDS</i> 2
Absorption correction	Integration (<i>X-RED32</i> ; Stoe & Cie, 2002)
<i>T_{min}</i> , <i>T_{max}</i>	0.664, 0.770
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	5748, 2125, 1709
<i>R_{int}</i>	0.033
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.628
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.034, 0.087, 1.02
No. of reflections	2125
No. of parameters	166
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.28, -0.38

Computer programs: *X-AREA* and *X-RED32* (Stoe & Cie, 2002), *SHELXS97* (Sheldrick, 2008), *SHELXL2017* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

obtained was dissolved in water and added to a aqueous solution of isonicotinamide (1.71 mmol, 0.21 g). The resulting suspension was filtered and the filtrate allowed to stand. Red prismatic crystals were obtained from the filtrate in five weeks.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The water and NH₂ H atoms were

located from difference-Fourier maps and freely refined. The C-bound H atoms were positioned geometrically and refined using a riding model: C–H = 0.93–0.97 Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Acknowledgements

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supporting information

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Synthesis, crystal structure and Hirshfeld surface analysis of tetraaquabis-(isonicotinamide- κN^1)cobalt(II) succinate

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Computing details

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA* (Stoe & Cie, 2002); data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2017* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2017* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

Tetraaquabis(isonicotinamide- κN^1)cobalt(II) butanedioate

Crystal data

$[\text{Co}(\text{C}_6\text{H}_6\text{N}_2\text{O})_2(\text{H}_2\text{O})_4](\text{C}_4\text{H}_4\text{O}_4)$

$M_r = 491.32$

Monoclinic, $P2_1/c$

$a = 9.6757$ (8) Å

$b = 10.0381$ (8) Å

$c = 11.4947$ (10) Å

$\beta = 112.489$ (6)°

$V = 1031.53$ (15) Å³

$Z = 2$

$F(000) = 510$

$D_x = 1.582$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 8789 reflections

$\theta = 3.1\text{--}30.2^\circ$

$\mu = 0.89$ mm⁻¹

$T = 296$ K

Prism, red

$0.68 \times 0.49 \times 0.37$ mm

Data collection

Stoe IPDS 2

diffractometer

Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus

Detector resolution: 6.67 pixels mm⁻¹

rotation method scans

Absorption correction: integration

(X-RED32; Stoe & Cie, 2002)

$T_{\min} = 0.664$, $T_{\max} = 0.770$

5748 measured reflections

2125 independent reflections

1709 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.033$

$\theta_{\max} = 26.5^\circ$, $\theta_{\min} = 4.0^\circ$

$h = -12 \rightarrow 12$

$k = -12 \rightarrow 12$

$l = -14 \rightarrow 10$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.034$

$wR(F^2) = 0.087$

$S = 1.02$

2125 reflections

166 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0544P)^2 + 0.0723P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$

$$\Delta\rho_{\max} = 0.28 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.38 \text{ e } \text{\AA}^{-3}$$

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.500000	0.500000	1.000000	0.02416 (13)
O3	0.40225 (19)	0.64528 (17)	0.85930 (16)	0.0323 (3)
O4	0.39411 (19)	0.34772 (15)	0.87503 (16)	0.0314 (3)
O2	0.44508 (19)	0.36520 (15)	0.66478 (15)	0.0372 (4)
O5	1.08679 (19)	0.30825 (16)	0.80841 (18)	0.0450 (4)
O1	0.2865 (2)	0.53407 (16)	0.62211 (16)	0.0413 (4)
N2	0.68645 (19)	0.47784 (15)	0.94294 (17)	0.0284 (4)
N1	1.0405 (3)	0.5081 (3)	0.7144 (3)	0.0523 (6)
C1	1.0166 (2)	0.4142 (2)	0.7847 (2)	0.0340 (5)
C2	0.9000 (2)	0.4398 (2)	0.8388 (2)	0.0291 (4)
C5	0.7381 (2)	0.5790 (2)	0.8958 (2)	0.0336 (5)
H5	0.700517	0.663743	0.898389	0.040*
C7	0.3809 (2)	0.4648 (2)	0.6004 (2)	0.0296 (4)
C3	0.8494 (3)	0.3354 (2)	0.8895 (2)	0.0348 (5)
H3	0.886482	0.249919	0.889455	0.042*
C6	0.8434 (2)	0.5649 (2)	0.8438 (2)	0.0343 (5)
H6	0.876190	0.638596	0.812443	0.041*
C4	0.7441 (3)	0.3579 (2)	0.9399 (2)	0.0353 (5)
H4	0.711309	0.286121	0.973646	0.042*
C8	0.4207 (3)	0.5013 (3)	0.4888 (3)	0.0535 (7)
H8A	0.368960	0.440472	0.420345	0.064*
H8B	0.382876	0.590118	0.461003	0.064*
H1A	0.982 (4)	0.584 (4)	0.697 (4)	0.083 (12)*
H1B	1.107 (4)	0.495 (3)	0.683 (4)	0.076 (11)*
H4A	0.403 (3)	0.355 (3)	0.812 (3)	0.035 (7)*
H3A	0.449 (3)	0.711 (3)	0.857 (3)	0.049 (8)*
H3B	0.373 (4)	0.612 (3)	0.792 (3)	0.055 (9)*
H4B	0.304 (4)	0.330 (3)	0.858 (3)	0.065 (10)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0267 (2)	0.02335 (19)	0.0296 (2)	-0.00065 (15)	0.01885 (15)	0.00042 (15)
O3	0.0388 (9)	0.0293 (8)	0.0331 (9)	-0.0031 (7)	0.0184 (7)	0.0019 (7)
O4	0.0343 (9)	0.0338 (8)	0.0335 (9)	-0.0035 (6)	0.0211 (7)	-0.0022 (6)
O2	0.0519 (10)	0.0311 (7)	0.0413 (9)	0.0079 (7)	0.0319 (8)	0.0046 (6)

O5	0.0432 (9)	0.0380 (9)	0.0700 (12)	-0.0002 (7)	0.0399 (9)	-0.0086 (8)
O1	0.0469 (9)	0.0431 (9)	0.0443 (10)	0.0117 (7)	0.0291 (8)	0.0043 (7)
N2	0.0296 (8)	0.0264 (9)	0.0373 (9)	-0.0010 (6)	0.0217 (7)	-0.0014 (7)
N1	0.0506 (12)	0.0602 (14)	0.0686 (15)	0.0086 (12)	0.0479 (12)	0.0121 (12)
C1	0.0285 (11)	0.0403 (12)	0.0406 (12)	-0.0040 (9)	0.0214 (10)	-0.0073 (9)
C2	0.0257 (10)	0.0333 (10)	0.0336 (11)	-0.0011 (8)	0.0174 (9)	-0.0032 (8)
C5	0.0368 (12)	0.0252 (10)	0.0475 (13)	0.0038 (8)	0.0260 (10)	0.0045 (9)
C7	0.0323 (10)	0.0304 (10)	0.0309 (11)	-0.0036 (8)	0.0175 (9)	-0.0010 (8)
C3	0.0368 (12)	0.0258 (10)	0.0515 (13)	-0.0003 (8)	0.0276 (10)	-0.0027 (9)
C6	0.0349 (11)	0.0320 (11)	0.0450 (13)	0.0004 (9)	0.0253 (10)	0.0076 (9)
C4	0.0400 (12)	0.0262 (10)	0.0516 (14)	-0.0018 (9)	0.0307 (11)	0.0014 (9)
C8	0.0439 (14)	0.0825 (19)	0.0455 (14)	0.0135 (14)	0.0298 (12)	0.0250 (14)

Geometric parameters (Å, °)

Co1—O4 ⁱ	2.0794 (16)	N1—H1A	0.92 (4)
Co1—O3	2.1134 (15)	N1—H1B	0.87 (4)
Co1—O4	2.0795 (16)	C1—C2	1.504 (3)
Co1—N2 ⁱ	2.1540 (16)	C2—C3	1.377 (3)
Co1—O3 ⁱ	2.1134 (15)	C2—C6	1.381 (3)
Co1—N2	2.1540 (16)	C5—C6	1.372 (3)
O3—H3A	0.81 (3)	C5—H5	0.9300
O3—H3B	0.79 (4)	C7—C8	1.519 (3)
O4—H4A	0.77 (3)	C3—C4	1.370 (3)
O4—H4B	0.83 (4)	C3—H3	0.9300
O2—C7	1.257 (3)	C6—H6	0.9300
O5—C1	1.235 (3)	C4—H4	0.9300
O1—C7	1.247 (3)	C8—C8 ⁱⁱ	1.456 (5)
N2—C4	1.333 (3)	C8—H8A	0.9700
N2—C5	1.334 (3)	C8—H8B	0.9700
N1—C1	1.317 (3)		
O3—Co1—O3 ⁱ	180	O5—C1—N1	122.8 (2)
O4 ⁱ —Co1—O4	180	O5—C1—C2	119.4 (2)
N2 ⁱ —Co1—N2	180	N1—C1—C2	117.8 (2)
O4 ⁱ —Co1—O3	88.82 (7)	C3—C2—C6	117.62 (18)
O4—Co1—O3	91.18 (7)	C3—C2—C1	119.32 (18)
O4 ⁱ —Co1—O3 ⁱ	91.18 (7)	C6—C2—C1	123.03 (19)
O4—Co1—O3 ⁱ	88.82 (7)	N2—C5—C6	123.66 (19)
O4 ⁱ —Co1—N2 ⁱ	87.85 (6)	N2—C5—H5	118.2
O4—Co1—N2 ⁱ	92.15 (7)	C6—C5—H5	118.2
O3—Co1—N2 ⁱ	88.85 (6)	O1—C7—O2	124.09 (19)
O3 ⁱ —Co1—N2 ⁱ	91.15 (6)	O1—C7—C8	118.4 (2)
O4 ⁱ —Co1—N2	92.15 (7)	O2—C7—C8	117.47 (19)
O4—Co1—N2	87.85 (6)	C4—C3—C2	119.73 (19)
O3—Co1—N2	91.15 (6)	C4—C3—H3	120.1
O3 ⁱ —Co1—N2	88.85 (6)	C2—C3—H3	120.1
Co1—O3—H3A	120 (2)	C5—C6—C2	118.99 (19)

Co1—O3—H3B	110 (2)	C5—C6—H6	120.5
H3A—O3—H3B	108 (3)	C2—C6—H6	120.5
Co1—O4—H4A	112 (2)	N2—C4—C3	123.14 (19)
Co1—O4—H4B	121 (2)	N2—C4—H4	118.4
H4A—O4—H4B	106 (3)	C3—C4—H4	118.4
C4—N2—C5	116.83 (17)	C8 ⁱⁱ —C8—C7	115.9 (3)
C4—N2—Co1	120.60 (13)	C8 ⁱⁱ —C8—H8A	108.3
C5—N2—Co1	122.14 (13)	C7—C8—H8A	108.3
C1—N1—H1A	119 (3)	C8 ⁱⁱ —C8—H8B	108.3
C1—N1—H1B	119 (2)	C7—C8—H8B	108.3
H1A—N1—H1B	122 (3)	H8A—C8—H8B	107.4
O5—C1—C2—C3	-14.5 (3)	N2—C5—C6—C2	0.2 (4)
N1—C1—C2—C3	166.3 (2)	C3—C2—C6—C5	-1.4 (3)
O5—C1—C2—C6	163.5 (2)	C1—C2—C6—C5	-179.5 (2)
N1—C1—C2—C6	-15.7 (3)	C5—N2—C4—C3	-1.2 (4)
C4—N2—C5—C6	1.1 (4)	Co1—N2—C4—C3	171.39 (19)
Co1—N2—C5—C6	-171.37 (19)	C2—C3—C4—N2	0.0 (4)
C6—C2—C3—C4	1.4 (4)	O1—C7—C8—C8 ⁱⁱ	136.1 (3)
C1—C2—C3—C4	179.5 (2)	O2—C7—C8—C8 ⁱⁱ	-44.5 (5)

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

Hydrogen-bond geometry (\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>
O3—H3B \cdots O1	0.79 (4)	1.97 (4)	2.756 (3)	176 (3)
O4—H4A \cdots O2	0.77 (3)	1.88 (3)	2.651 (2)	174 (3)
O3—H3A \cdots O2 ⁱⁱⁱ	0.81 (3)	1.92 (3)	2.729 (2)	175 (3)
O4—H4B \cdots O5 ^{iv}	0.83 (4)	1.97 (4)	2.801 (2)	174 (3)
N1—H1A \cdots O5 ^v	0.92 (4)	2.34 (4)	3.227 (3)	160 (3)
N1—H1B \cdots O1 ^{vi}	0.87 (4)	2.14 (4)	2.966 (3)	160 (3)
C5—H5 \cdots O2 ⁱⁱⁱ	0.93	2.41	3.307 (3)	161
C6—H6 \cdots O5 ^v	0.93	2.31	3.223 (3)	167

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