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catena-Poly[[[bis(2-methyl-1*H*-imidazole)cobalt(II)]-μ-cyclohexane-1,4-dicarboxylato] monohydrate]

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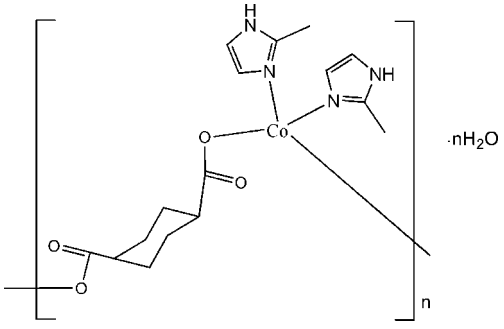
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.041; wR factor = 0.094; data-to-parameter ratio = 17.5.

In the title compound, $\{[Co(1,4\text{-chdc})(L)_2]\cdot H_2O\}_n$, where 1,4-chdc is the cyclohexane-1,4-dicarboxylate dianion, $C_8H_{10}O_4^{2-}$, and L is 2-methyl-1*H*-imidazole, $C_4H_6N_2$, each Co^{II} atom is four-coordinated by two O atoms from two 1,4-chdc ligands and two N atoms from two L molecules in a distorted tetrahedral geometry. Each 1,4-chdc anion acts as a bidentate ligand that links two Co^{II} atoms, thus generating a helical chain. These chains are decorated with L ligands alternately on the two sides. In addition, O—H···O and N—H···O hydrogen bonds complete the structure of (I).

Related literature

Two isomorphous structures (Qi *et al.*, 2003) of coordination polymers with cyclohexane-1,4-dicarboxylate (1,4-chdc) have been reported, *viz.* $[Co_2(phen)_2(1,4\text{-chdc})_2(H_2O)_2]_n$ and $[Ni_2(phen)_2(1,4\text{-chdc})_2(H_2O)_2]_n$ (phen is 1,10-phenanthroline). The striking feature of the two compounds is that they both exhibit an infinite helical chain-like structure with 2_1 helices.

For related literature, see: Chen & Liu (2002); Zhang *et al.* (2007).



Experimental

Crystal data

$[Co(C_8H_{10}O_4)(C_4H_6N_2)_2]\cdot H_2O$
M_r = 411.32
Monoclinic, $P2_1/c$
a = 13.300 (3) Å
b = 11.075 (2) Å
c = 14.334 (3) Å
β = 116.82 (3)°
V = 1884.2 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.95 mm^{-1}
T = 293 (2) K
0.29 × 0.27 × 0.24 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.752, T_{max} = 0.798
15286 measured reflections
4295 independent reflections
3311 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.094
S = 1.06
4295 reflections
245 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—N1	2.0460 (19)	Co1—O1	1.955 (2)
Co1—N3	2.024 (2)	Co1—O3^{i}	2.0042 (16)
O1—Co1—O3^{i}	97.93 (8)	O1—Co1—N1	107.66 (9)
O1—Co1—N3	132.04 (9)	O3^{i}—Co1—N1	106.51 (7)
O3^{i}—Co1—N3	107.31 (8)	N3—Co1—N1	103.32 (8)

Symmetry code: (i) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—HW11···O2^{ii}	0.826 (17)	1.904 (18)	2.723 (3)	171 (3)
O1W—HW12···O3^{iii}	0.837 (16)	1.962 (16)	2.790 (3)	170 (3)
N2—H2···O4^{iv}	0.86	1.98	2.827 (3)	168
N4—H4···O1W	0.86	1.84	2.685 (3)	169

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2125).

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Zhang, Y.-M., Hou, D.-Y., Xin, G. & Li, T.-C. (2007). *Acta Cryst.* E**63**, m1363–m1364.

supplementary materials

Acta Cryst. (2007). E**63**, m1735-m1736 [**doi:10.1107/S1600536807024063**]

catena-Poly[[[bis(2-methyl-1*H*-imidazole)cobalt(II)]-μ-cyclohexane-1,4-dicarboxylato] monohydrate]

Y.-M. Zhang, G. Xin, Dong-Yan Hou and T.-C. Li

Comment

Helical structures have received much attention in coordination chemistry (Chen & Liu, 2002). The flexible bidentate organic acid may be useful in the generation of helical chains in the presence of secondary ligands (Zhang *et al.*, 2007). The N atoms from the secondary ligand may occupy one or two coordination positions of metal ions. The rest of the coordination positions are available for other carboxylate ligands to allow the formation of a helical structure. Here, we selected cyclohexane-1,4-dicarboxylic acid (1,4-chdcH_2) as a organic acid ligand and 2-methyl-1*H*-imidazole (*L*) as a secondary ligand, resulting in a new helical chain structure, [Co(1,4-chdc)(*L*)$_2$]·H_2O, (I), which is reported.

Selected bond lengths and angles for (I) are given in Table 1. In compound (I), each Co(II) atom is four-coordinated by two O atoms from two 1,4-chdc ligands, and two N atoms from two *L* molecules in a distorted tetrahedral geometry (Fig. 1). The Co1—O1 and Co1—O3^{i} distances are 1.955 (2) and 2.0042 (16) Å, respectively (Table 1). The Co1—N1 and Co1—N4 distances are 2.0460 (19) and 2.024 (2) Å, respectively (Table 1). Each 1,4-chdc ligand links two neighboring Co(II) atoms in a bidentate mode, generating a unique helical chain (Fig. 2). These chains are decorated with *L* ligands alternately at two sides. Finally, the O—H···O and N—H···O hydrogen bonds complete the structure of (I).

Experimental

A mixture of $CoCl_2$·$2H_2O$ (0.5 mmol), 1,4-chdc acid (0.5 mmol), and *L* (0.5 mmol) was adjusted to pH=6.5 by addition of aqueous NaOH solution. The resulting solution was filtered, the filtrate was allowed to stand in air at room temperature for one week, and the pink crystals of (I) were obtained (yield 39% based on Co).

Refinement

All H atoms on C and N atoms were positioned geometrically (N—H = 0.86 Å and C—H = 0.93 Å) and refined as riding, with U_{iso}(H)=1.2U_{eq}(carrier). The water H-atoms were located in a difference Fourier map, and were refined with distance restraints of O–H = 0.85 Å.

Figures

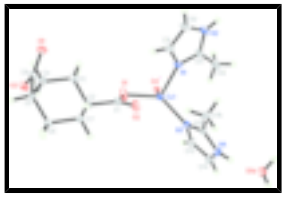

Fig. 1. The structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Symmetry code: (i) $1-x, y-1/2, 1.5-z$.

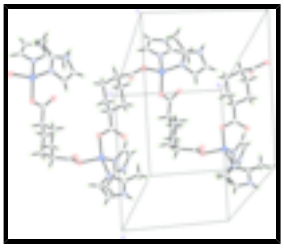

Fig. 2. View of the helical chain structure of (I).

catena-Poly[[[bis(2-methyl-1_H_-imidazole)cobalt(II)] -μ-cyclohexane-1,4-dicarboxylato] monohydrate]

Crystal data

$[Co(C_8H_{10}O_4)(C_4H_6N_2)_2]\cdot H_2O$	F_{000} = 860
M_r = 411.32	D_x = 1.450 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 11934 reflections
a = 13.300 (3) Å	θ = 3.2–27.5º
b = 11.075 (2) Å	μ = 0.95 mm^{-1}
c = 14.334 (3) Å	T = 293 (2) K
β = 116.82 (3)º	Block, pink
V = 1884.2 (8) Å^3	0.29 × 0.27 × 0.24 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	4295 independent reflections
Radiation source: rotating anode	3311 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.046
Detector resolution: 10.0 pixels mm^{-1}	θ_{max} = 27.5º
T = 293(2) K	θ_{min} = 3.2º
ω scan	h = −15→17
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	k = −14→14
T_{min} = 0.752, T_{max} = 0.798	l = −18→16
15286 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.041	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.094	$w = 1/[\sigma^2(F_o^2) + (0.039P)^2 + 0.6548P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max}$ = 0.001

4295 reflections	$\Delta\rho_{max} = 0.37$ e Å^{-3}
245 parameters	$\Delta\rho_{min} = -0.25$ e Å^{-3}
3 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
C1	0.4008 (2)	0.2780 (2)	0.71383 (18)	0.0401 (6)
C2	0.4978 (2)	0.2657 (2)	0.68613 (18)	0.0360 (5)
H2A	0.4889	0.1873	0.6516	0.043*
C3	0.6113 (2)	0.2625 (2)	0.78389 (18)	0.0410 (6)
H3A	0.6228	0.3382	0.8214	0.049*
H3B	0.6109	0.1981	0.8295	0.049*
C4	0.7079 (2)	0.2425 (2)	0.7561 (2)	0.0432 (6)
H4A	0.7022	0.1617	0.7280	0.052*
H4B	0.7788	0.2479	0.8192	0.052*
C5	0.7085 (2)	0.3338 (2)	0.67631 (17)	0.0327 (5)
H5	0.7632	0.3054	0.6529	0.039*
C6	0.5928 (2)	0.3373 (2)	0.58001 (17)	0.0386 (6)
H6A	0.5928	0.4003	0.5330	0.046*
H6B	0.5796	0.2609	0.5433	0.046*
C7	0.4978 (2)	0.3608 (2)	0.60950 (17)	0.0374 (5)
H7A	0.5072	0.4402	0.6409	0.045*
H7B	0.4261	0.3593	0.5471	0.045*
C8	0.74491 (19)	0.4602 (2)	0.72160 (17)	0.0319 (5)
C9	0.3517 (2)	0.4190 (2)	0.92264 (19)	0.0464 (6)
H9	0.4015	0.4346	0.8948	0.056*
C10	0.3467 (3)	0.4798 (3)	1.0017 (2)	0.0540 (8)
H10	0.3919	0.5445	1.0383	0.065*
C11	0.2184 (2)	0.3384 (2)	0.94879 (17)	0.0397 (6)
C12	0.1208 (3)	0.2644 (3)	0.9383 (3)	0.0629 (8)
H12A	0.0613	0.3166	0.9342	0.094*
H12B	0.1434	0.2123	0.9979	0.094*
H12C	0.0946	0.2165	0.8759	0.094*

C13	0.0093 (2)	0.1407 (2)	0.6170 (2)	0.0453 (6)
H13	0.0239	0.0583	0.6269	0.054*
C14	−0.0897 (2)	0.1900 (3)	0.5501 (2)	0.0553 (7)
H14	−0.1549	0.1491	0.5056	0.066*
C15	0.0311 (2)	0.3347 (2)	0.63310 (17)	0.0347 (5)
C16	0.0767 (2)	0.4585 (2)	0.6651 (2)	0.0508 (7)
H16A	0.0327	0.5147	0.6110	0.076*
H16B	0.1535	0.4609	0.6766	0.076*
H16C	0.0732	0.4800	0.7285	0.076*
N1	0.27049 (17)	0.32969 (17)	0.88959 (14)	0.0362 (5)
N2	0.2633 (2)	0.42856 (19)	1.01784 (15)	0.0485 (6)
H2	0.2427	0.4501	1.0643	0.058*
N3	0.08621 (16)	0.23135 (16)	0.66915 (14)	0.0338 (4)
N4	−0.07494 (17)	0.3123 (2)	0.56069 (16)	0.0445 (5)
H4	−0.1250	0.3658	0.5268	0.053*
O1	0.3881 (2)	0.19246 (18)	0.76549 (19)	0.0648 (6)
O2	0.33529 (19)	0.3642 (2)	0.68658 (16)	0.0742 (7)
O1W	−0.23698 (18)	0.48020 (19)	0.47705 (16)	0.0562 (5)
O3	0.74594 (15)	0.54197 (14)	0.65811 (12)	0.0387 (4)
O4	0.77284 (16)	0.48266 (16)	0.81481 (13)	0.0480 (5)
Co1	0.24756 (3)	0.20400 (3)	0.77712 (2)	0.03035 (10)
HW12	−0.249 (2)	0.503 (2)	0.5266 (16)	0.054 (9)*
HW11	−0.271 (3)	0.521 (3)	0.4237 (16)	0.077 (11)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0397 (14)	0.0493 (15)	0.0358 (12)	−0.0085 (12)	0.0209 (11)	−0.0083 (11)
C2	0.0381 (13)	0.0353 (12)	0.0393 (12)	−0.0057 (10)	0.0216 (10)	−0.0058 (10)
C3	0.0417 (14)	0.0449 (14)	0.0376 (13)	0.0004 (11)	0.0190 (11)	0.0097 (11)
C4	0.0386 (14)	0.0353 (12)	0.0543 (15)	0.0063 (11)	0.0198 (12)	0.0078 (11)
C5	0.0336 (12)	0.0315 (11)	0.0394 (12)	−0.0013 (9)	0.0221 (10)	−0.0063 (9)
C6	0.0436 (15)	0.0450 (13)	0.0310 (11)	−0.0108 (11)	0.0203 (11)	−0.0070 (10)
C7	0.0322 (13)	0.0462 (14)	0.0306 (11)	−0.0018 (11)	0.0112 (10)	0.0010 (10)
C8	0.0304 (12)	0.0341 (12)	0.0344 (11)	−0.0029 (10)	0.0175 (9)	−0.0047 (9)
C9	0.0522 (17)	0.0449 (15)	0.0409 (13)	−0.0072 (12)	0.0201 (12)	−0.0042 (11)
C10	0.069 (2)	0.0444 (15)	0.0386 (14)	−0.0037 (14)	0.0160 (13)	−0.0106 (11)
C11	0.0526 (16)	0.0381 (13)	0.0303 (11)	0.0099 (11)	0.0205 (11)	0.0046 (10)
C12	0.077 (2)	0.066 (2)	0.0678 (19)	−0.0042 (17)	0.0528 (18)	−0.0046 (15)
C13	0.0416 (15)	0.0364 (14)	0.0538 (15)	−0.0033 (11)	0.0178 (12)	0.0026 (11)
C14	0.0375 (15)	0.0544 (18)	0.0625 (17)	−0.0095 (13)	0.0125 (13)	−0.0024 (14)
C15	0.0363 (13)	0.0384 (12)	0.0335 (11)	0.0039 (10)	0.0195 (10)	0.0020 (9)
C16	0.0540 (17)	0.0361 (14)	0.0571 (16)	0.0071 (12)	0.0206 (13)	0.0013 (12)
N1	0.0447 (12)	0.0351 (10)	0.0295 (10)	0.0014 (9)	0.0174 (9)	−0.0018 (8)
N2	0.0738 (17)	0.0435 (12)	0.0314 (10)	0.0133 (12)	0.0264 (11)	−0.0012 (9)
N3	0.0343 (10)	0.0319 (10)	0.0345 (10)	0.0025 (8)	0.0149 (8)	0.0012 (8)
N4	0.0337 (11)	0.0502 (13)	0.0471 (12)	0.0109 (10)	0.0160 (9)	0.0083 (10)
O1	0.0752 (15)	0.0534 (12)	0.0987 (16)	−0.0031 (11)	0.0682 (14)	0.0062 (11)

O2	0.0662 (14)	0.1131 (19)	0.0603 (12)	0.0437 (14)	0.0436 (11)	0.0330 (13)
O1W	0.0605 (13)	0.0701 (14)	0.0449 (11)	0.0277 (11)	0.0298 (10)	0.0136 (10)
O3	0.0531 (11)	0.0310 (8)	0.0398 (9)	−0.0039 (7)	0.0279 (8)	−0.0035 (7)
O4	0.0548 (12)	0.0573 (11)	0.0340 (9)	−0.0179 (9)	0.0219 (8)	−0.0143 (8)
Co1	0.03402 (18)	0.03078 (16)	0.02738 (16)	0.00234 (13)	0.01485 (12)	0.00074 (12)

Geometric parameters (Å, °)

C1—O2	1.231 (3)	C10—H10	0.9300
C1—O1	1.260 (3)	C11—N1	1.319 (3)
C1—C2	1.518 (4)	C11—N2	1.342 (3)
C2—C7	1.521 (3)	C11—C12	1.484 (4)
C2—C3	1.528 (3)	C12—H12A	0.9600
C2—H2A	0.9800	C12—H12B	0.9600
C3—C4	1.523 (4)	C12—H12C	0.9600
C3—H3A	0.9700	C13—C14	1.346 (4)
C3—H3B	0.9700	C13—N3	1.387 (3)
C4—C5	1.530 (3)	C13—H13	0.9300
C4—H4A	0.9700	C14—N4	1.367 (3)
C4—H4B	0.9700	C14—H14	0.9300
C5—C8	1.526 (3)	C15—N3	1.332 (3)
C5—C6	1.536 (3)	C15—N4	1.344 (3)
C5—H5	0.9800	C15—C16	1.486 (3)
C6—C7	1.524 (3)	C16—H16A	0.9600
C6—H6A	0.9700	C16—H16B	0.9600
C6—H6B	0.9700	C16—H16C	0.9600
C7—H7A	0.9700	Co1—N1	2.0460 (19)
C7—H7B	0.9700	N2—H2	0.8600
C8—O4	1.240 (3)	Co1—N3	2.024 (2)
C8—O3	1.289 (3)	N4—H4	0.8600
C9—C10	1.346 (4)	Co1—O1	1.955 (2)
C9—N1	1.382 (3)	O1W—HW12	0.837 (16)
C9—H9	0.9300	O1W—HW11	0.826 (17)
C10—N2	1.356 (4)	Co1—O3^{i}	2.0042 (16)
O2—C1—O1	120.4 (3)	N2—C10—H10	126.6
O2—C1—C2	123.4 (2)	N1—C11—N2	110.0 (2)
O1—C1—C2	116.2 (2)	N1—C11—C12	125.7 (2)
C1—C2—C7	113.8 (2)	N2—C11—C12	124.3 (2)
C1—C2—C3	111.52 (19)	C11—C12—H12A	109.5
C7—C2—C3	110.88 (19)	C11—C12—H12B	109.5
C1—C2—H2A	106.7	H12A—C12—H12B	109.5
C7—C2—H2A	106.7	C11—C12—H12C	109.5
C3—C2—H2A	106.7	H12A—C12—H12C	109.5
C4—C3—C2	111.4 (2)	H12B—C12—H12C	109.5
C4—C3—H3A	109.4	C14—C13—N3	109.7 (2)
C2—C3—H3A	109.4	C14—C13—H13	125.2
C4—C3—H3B	109.4	N3—C13—H13	125.2
C2—C3—H3B	109.4	C13—C14—N4	106.1 (2)
H3A—C3—H3B	108.0	C13—C14—H14	126.9

C3—C4—C5	112.9 (2)	N4—C14—H14	126.9
C3—C4—H4A	109.0	N3—C15—N4	110.0 (2)
C5—C4—H4A	109.0	N3—C15—C16	126.6 (2)
C3—C4—H4B	109.0	N4—C15—C16	123.3 (2)
C5—C4—H4B	109.0	C15—C16—H16A	109.5
H4A—C4—H4B	107.8	C15—C16—H16B	109.5
C8—C5—C4	113.31 (19)	H16A—C16—H16B	109.5
C8—C5—C6	110.85 (19)	C15—C16—H16C	109.5
C4—C5—C6	110.3 (2)	H16A—C16—H16C	109.5
C8—C5—H5	107.4	H16B—C16—H16C	109.5
C4—C5—H5	107.4	C11—N1—C9	106.5 (2)
C6—C5—H5	107.4	C11—N1—Co1	128.45 (18)
C7—C6—C5	112.02 (18)	C9—N1—Co1	124.96 (18)
C7—C6—H6A	109.2	C11—N2—C10	108.2 (2)
C5—C6—H6A	109.2	C11—N2—H2	125.9
C7—C6—H6B	109.2	C10—N2—H2	125.9
C5—C6—H6B	109.2	C15—N3—C13	105.7 (2)
H6A—C6—H6B	107.9	C15—N3—Co1	129.33 (16)
C2—C7—C6	110.6 (2)	C13—N3—Co1	125.00 (16)
C2—C7—H7A	109.5	C15—N4—C14	108.5 (2)
C6—C7—H7A	109.5	C15—N4—H4	125.8
C2—C7—H7B	109.5	C14—N4—H4	125.8
C6—C7—H7B	109.5	C1—O1—Co1	112.82 (19)
H7A—C7—H7B	108.1	HW12—O1W—HW11	113 (2)
O4—C8—O3	121.7 (2)	C8—O3—Co1^{ii}	108.32 (14)
O4—C8—C5	121.7 (2)	O1—Co1—O3^{i}	97.93 (8)
O3—C8—C5	116.51 (18)	O1—Co1—N3	132.04 (9)
C10—C9—N1	108.6 (3)	O3^{i}—Co1—N3	107.31 (8)
C10—C9—H9	125.7	O1—Co1—N1	107.66 (9)
N1—C9—H9	125.7	O3^{i}—Co1—N1	106.51 (7)
C9—C10—N2	106.8 (2)	N3—Co1—N1	103.32 (8)
C9—C10—H10	126.6		
O2—C1—C2—C7	−7.7 (3)	N4—C15—N3—C13	−0.9 (3)
O1—C1—C2—C7	170.7 (2)	C16—C15—N3—C13	179.6 (3)
O2—C1—C2—C3	118.6 (3)	N4—C15—N3—Co1	179.31 (16)
O1—C1—C2—C3	−63.0 (3)	C16—C15—N3—Co1	−0.2 (4)
C1—C2—C3—C4	176.5 (2)	C14—C13—N3—C15	0.7 (3)
C7—C2—C3—C4	−55.5 (3)	C14—C13—N3—Co1	−179.42 (19)
C2—C3—C4—C5	53.8 (3)	N3—C15—N4—C14	0.7 (3)
C3—C4—C5—C8	72.4 (3)	C16—C15—N4—C14	−179.8 (3)
C3—C4—C5—C6	−52.6 (3)	C13—C14—N4—C15	−0.2 (3)
C8—C5—C6—C7	−72.2 (2)	O2—C1—O1—Co1	8.0 (3)
C4—C5—C6—C7	54.1 (3)	C2—C1—O1—Co1	−170.51 (16)
C1—C2—C7—C6	−176.17 (19)	O4—C8—O3—Co1^{ii}	−16.5 (3)
C3—C2—C7—C6	57.1 (3)	C5—C8—O3—Co1^{ii}	164.01 (15)
C5—C6—C7—C2	−57.0 (3)	C1—O1—Co1—O3^{i}	171.49 (18)
C4—C5—C8—O4	1.4 (3)	C1—O1—Co1—N3	49.5 (2)

C6—C5—C8—O4	126.1 (2)	C1—O1—Co1—N1	−78.3 (2)
C4—C5—C8—O3	−179.2 (2)	C15—N3—Co1—O1	−87.9 (2)
C6—C5—C8—O3	−54.5 (3)	C13—N3—Co1—O1	92.3 (2)
N1—C9—C10—N2	0.1 (3)	C15—N3—Co1—O3^{i}	153.67 (19)
N3—C13—C14—N4	−0.3 (3)	C13—N3—Co1—O3^{i}	−26.1 (2)
N2—C11—N1—C9	−0.3 (3)	C15—N3—Co1—N1	41.4 (2)
C12—C11—N1—C9	176.8 (3)	C13—N3—Co1—N1	−138.4 (2)
N2—C11—N1—Co1	175.74 (15)	C11—N1—Co1—O1	−154.1 (2)
C12—C11—N1—Co1	−7.1 (4)	C9—N1—Co1—O1	21.3 (2)
C10—C9—N1—C11	0.1 (3)	C11—N1—Co1—O3^{i}	−49.9 (2)
C10—C9—N1—Co1	−176.08 (18)	C9—N1—Co1—O3^{i}	125.47 (19)
N1—C11—N2—C10	0.3 (3)	C11—N1—Co1—N3	63.0 (2)
C12—C11—N2—C10	−176.8 (3)	C9—N1—Co1—N3	−121.63 (19)
C9—C10—N2—C11	−0.3 (3)		

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+3/2; (ii) −*x*+1, *y*+1/2, −*z*+3/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—HW11···O2^{iii}	0.826 (17)	1.904 (18)	2.723 (3)	171 (3)
O1W—HW12···O3^{iv}	0.837 (16)	1.962 (16)	2.790 (3)	170 (3)
N2—H2···O4^{v}	0.86	1.98	2.827 (3)	168
N4—H4···O1W	0.86	1.84	2.685 (3)	169

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

Fig. 1

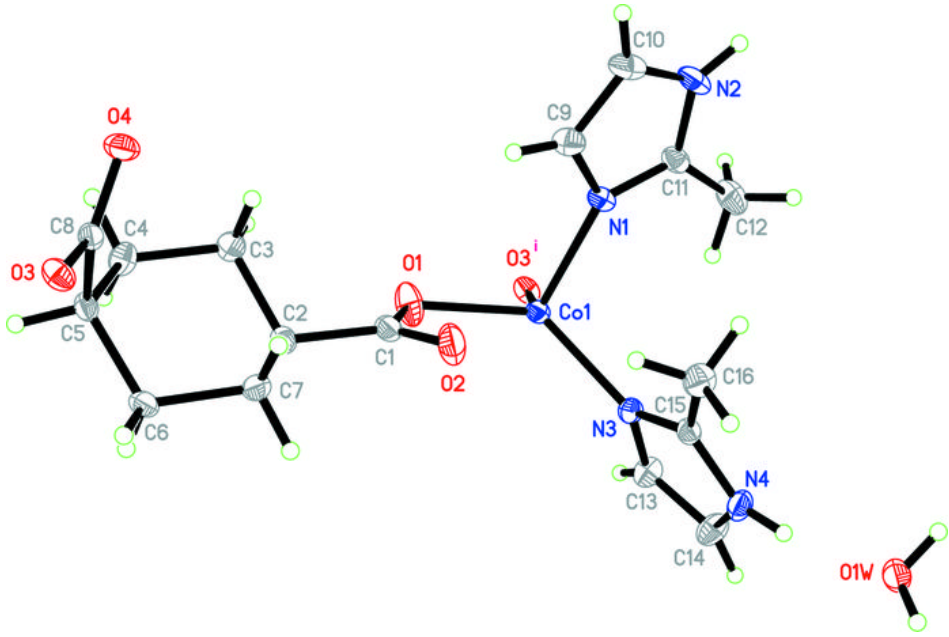
C10
N2
C9
C11
O4
C8
C4
C3
N1
C12
O3
O1
O3 i
C2
Co1
C5
C1
O2
C16
C7
C15
N3
C6
N4
C13
C14
O1W

Fig. 2