metal-organic compounds

catena-Poly[[cobalt(II)-μ-[N,N′-1,3-bis-(imidazol-1-ylmethyl)benzene]-κ²N³:N³′-μ-(5-carboxybenzene-1,3-dicarboxylato)-κ²O¹:O³] monohydrate]

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The title Co^{II} coordination polymer, $\{[Co(C_9H_4O_6)(C_{14}H_{14}N_4)]\cdot H_2O\}_n$, was obtained by reaction of $Co(NO_3)_2\cdot 6H_2O$, benzene-1,3,5-tricarboxylic acid (H_3BTC) and 1,3-bis(imidazol-1-ylmethyl)benzene (L). Each Co^{II} cation is four-coordinated by an O_2N_2 donor set in a distorted tetrahedral geometry. The Co^{II} centers are connected into a one-dimensional double-stranded chain by HBTC anions and L ligands. The chains are further connected through hydrogen-bonding interactions between the hydroxyl groups of adjacent HBTC anions and face-to-face π–π interactions between the benzene rings of adjacent L ligands [average face-to-face distance of 3.427 (3) Å], resulting in the formation of a three-dimensional supramolecular structure.

Related literature

For related crystal structures, see Liu *et al.* (2007) and Xie *et al.* (2007).
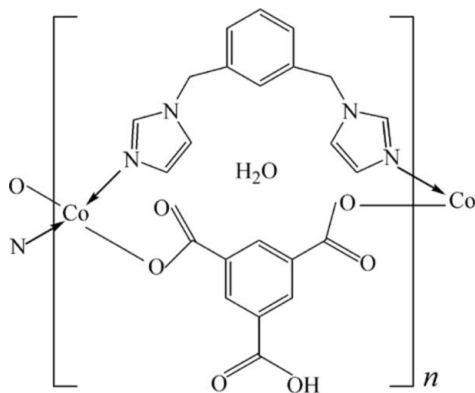
Experimental

Crystal data

$[Co(C_9H_4O_6)(C_{14}H_{14}N_4)]\cdot H_2O$	V = 2159.21 (18) Å³
M_r = 523.36	Z = 4
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
a = 7.8535 (4) Å	μ = 0.85 mm^{-1}
b = 16.5308 (7) Å	T = 293 (2) K
c = 16.7344 (8) Å	$0.13 \times 0.11 \times 0.09$ mm
β = 96.350 (1)°	

Data collection

Bruker APEX CCD area-detector diffractometer	13208 measured reflections
Absorption correction: multi-scan ($SADABS$; Sheldrick, 1996)	5192 independent reflections
T_{min} = 0.85, T_{max} = 0.88	3606 reflections with $I > 2\sigma(I)$
(expected range = 0.895–0.926)	R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.136	
S = 1.04	
5192 reflections	$\Delta\rho_{max}$ = 0.53 e Å^{-3}
322 parameters	$\Delta\rho_{min}$ = -0.76 e Å^{-3}
3 restraints	

Table 1
Selected geometric parameters (Å, °).

Co1—O6^i	1.968 (2)	Co1—N1	2.026 (2)
Co1—O2	2.024 (2)	Co1—N4^i	2.057 (2)
O6^i—Co1—O2	103.70 (9)	O6^i—Co1—N4^i	94.21 (9)
O6^i—Co1—N1	111.27 (9)	O2—Co1—N4^i	110.41 (9)
O2—Co1—N1	127.96 (9)	N1—Co1—N4^i	104.23 (9)

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1W—H1$A\cdots$O1	0.93 (2)	1.74 (3)	2.657 (5)	166 (9)
O4—H4$A\cdots$O3^{ii}	0.82	1.87	2.680 (3)	173

Symmetry code: (ii) $-x + 3, -y + 1, -z + 1$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; 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 materials

catena-Poly[[cobalt(II)-$^{\mu}$-[*N,N'*-1,3-bis(imidazol-1-ylmethyl)benzene]-$\kappa^2N^3:N^{3'}$-$^{\mu}$-(5-carboxybenzene-1,3-dicarboxylato)-$\kappa^2O^1:O^3$] monohydrate]

Y.-Y. Liu, J.-F. Ma and G.-H. Wei

Comment

As part of an investigation of the transition metal application there is a need to prepare further examples of these compounds. In this paper, the structure of the title compound, (I), is described.

As shown in Fig. 1, the Co^{II} ions is coordinated by two oxygen atoms from two HBTC anions and two nitrogen atoms from two *L* ligands. Each Co^{II} cation has a distorted tetrahedral coordination geometry. As illustrated in Fig. 2, each *L* ligand in (I) coordinates to two Co^{II} cations, thus acting as a bridging bidentate ligand. The Co^{II} cations are bridged by HBTC anions and *L* ligands to form a double-stranded chain, with the interchain Co⋯Co distance of 9.072 (6) Å. The hydroxyl groups of adjacent HBTC anions are involved in hydrogen bonding interactions. There also exist face-to-face π-π interactions between the benzene rings of *L* ligands of adjacent double-stranded chains (with centroid-to-centriod distance of 3.905 (2) Å, and average face-to-face distances of 3.427 (3) Å). These noncovalent interactions connect the whole structure to a 3-D supramolecular framework (Fig. 3). The lattice water molecule connects with HBTC anion *via* hydrogen bond.

Experimental

The ligand *L* was synthesized according to the literature (Liu *et al.*, 2007). A mixture of Co(NO$_3$)$_2$·6H$_2$O (0.11 g, 0.4 mmol), H$_3$BTC (0.10 g, 0.45 mmol), *L* (0.10 g, 0.4 mmol) and water (7 ml) was stirred for 10 min in air. The mixture was sealed in a Teflon reactor (15 ml) and heated at 180 °C for 3 days. After the mixture had been cooled to room temperature at 10 °C.h^{-1}, purple crystals of (I) were obtained. Yield: 30%.

Refinement

The C-bound and hydroxy H-atoms were geometrically positioned (C—H 0.93–0.97 Å, O—H 0.82 Å) and refined using a riding model, with U_{iso} = 1.2–1.5U_{eq} (C, O). Water H atoms were located in a difference Fourier map and refined as riding atoms with U_{iso}(H) = 1.5U_{eq}(O).
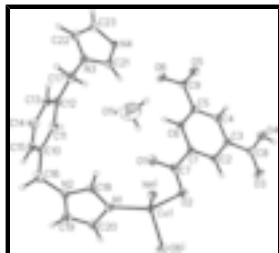
supplementary materials

Figures

Fig. 1. A view of the local coordination of the Co^{II} cation in (I) showing the atomic numbering [symmetry code: (i) $x + 1/2, -y + 1/2, z + 1/2$]. Displacement ellipsoids are drawn at the 30% probability level.
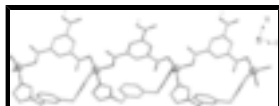
Fig. 2. Schematic view of the double-stranded chain in (I).
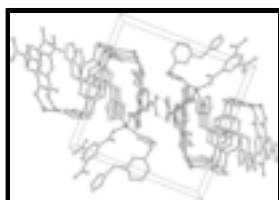
Fig. 3. The packing diagram of (I). The hydrogen bonding interactions are indicated by dotted lines. H atoms omitted for clarity.

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Crystal data

[Co(C$_9$H$_4$O$_6$)(C$_{14}$H$_{14}$N$_4$)]·H$_2$O	F_{000} = 1076
M_r = 523.36	D_x = 1.610 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: not measured K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation λ = 0.71069 Å
a = 7.8535 (4) Å	Cell parameters from 3606 reflections
b = 16.5308 (7) Å	θ = 1.7–28.3º
c = 16.7344 (8) Å	μ = 0.85 mm^{-1}
β = 96.3500 (10)º	T = 293 (2) K
V = 2159.21 (18) Å^3	Block, purple
Z = 4	0.13 × 0.11 × 0.09 mm

Data collection

Bruker APEX CCD area-detector diffractometer	5192 independent reflections
Radiation source: fine-focus sealed tube	3606 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.046
T = 293(2) K	θ_{max} = 28.3º
ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −10→10

$T_{min} = 0.85$, $T_{max} = 0.88$	$k = -22 \rightarrow 11$
13208 measured reflections	$l = -20 \rightarrow 21$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.136$	$w = 1/[\sigma^2(F_o^2) + (0.069P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
5192 reflections	$\Delta\rho_{max} = 0.53$ e Å^{-3}
322 parameters	$\Delta\rho_{min} = -0.76$ 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}
Co1	0.91070 (5)	0.18840 (2)	0.78370 (2)	0.02526 (13)
C1	0.9365 (4)	0.31872 (16)	0.58113 (17)	0.0268 (6)
C2	1.0894 (4)	0.36035 (17)	0.57876 (16)	0.0280 (6)
H2	1.1715	0.3605	0.6233	0.034*
C3	1.1189 (3)	0.40177 (17)	0.50920 (16)	0.0270 (6)
C4	0.9958 (3)	0.40212 (17)	0.44239 (16)	0.0267 (6)
H4	1.0159	0.4304	0.3963	0.032*
C5	0.8430 (3)	0.36021 (17)	0.44470 (16)	0.0261 (6)
C6	0.8149 (4)	0.31896 (17)	0.51446 (17)	0.0280 (6)
H6	0.7127	0.2910	0.5164	0.034*
C7	0.9062 (4)	0.26952 (17)	0.65377 (17)	0.0295 (6)
C8	1.2853 (4)	0.44426 (18)	0.50588 (17)	0.0321 (7)
C9	0.7107 (4)	0.35829 (17)	0.37216 (16)	0.0291 (6)
C10	0.3481 (4)	−0.02287 (17)	0.62968 (18)	0.0298 (6)

C11	0.2631 (4)	0.04946 (18)	0.61044 (18)	0.0315 (7)
H11	0.2456	0.0857	0.6512	0.038*
C12	0.2038 (4)	0.06864 (18)	0.53144 (18)	0.0322 (7)
C13	0.2269 (4)	0.01358 (19)	0.47063 (19)	0.0359 (7)
H13	0.1864	0.0254	0.4176	0.043*
C14	0.3102 (4)	−0.0589 (2)	0.48938 (19)	0.0389 (7)
H14	0.3265	−0.0954	0.4486	0.047*
C15	0.3694 (4)	−0.07736 (19)	0.56790 (19)	0.0338 (7)
H15	0.4240	−0.1265	0.5798	0.041*
C16	0.4167 (4)	−0.04058 (18)	0.71596 (18)	0.0348 (7)
H16A	0.3418	−0.0165	0.7517	0.042*
H16B	0.4181	−0.0986	0.7247	0.042*
C17	0.1128 (4)	0.1487 (2)	0.5173 (2)	0.0424 (8)
H17A	−0.0070	0.1414	0.5246	0.051*
H17B	0.1610	0.1869	0.5576	0.051*
C18	0.6342 (4)	0.06991 (18)	0.74057 (18)	0.0334 (7)
H18	0.5559	0.1122	0.7343	0.040*
C19	0.7410 (4)	−0.05168 (19)	0.74705 (17)	0.0350 (7)
H19	0.7518	−0.1077	0.7463	0.042*
C20	0.8687 (4)	0.00252 (18)	0.76034 (19)	0.0354 (7)
H20	0.9845	−0.0100	0.7706	0.042*
C21	0.2584 (4)	0.22522 (18)	0.41509 (18)	0.0315 (6)
H21	0.3587	0.2352	0.4486	0.038*
C22	0.0010 (4)	0.18314 (19)	0.3727 (2)	0.0370 (7)
H22	−0.1069	0.1596	0.3705	0.044*
C23	0.0662 (4)	0.22343 (19)	0.31230 (19)	0.0347 (7)
H23	0.0103	0.2319	0.2610	0.042*
N1	0.8011 (3)	0.07952 (15)	0.75631 (14)	0.0309 (5)
N2	0.5918 (3)	−0.00812 (14)	0.73483 (14)	0.0293 (5)
N3	0.1237 (3)	0.18368 (15)	0.43720 (16)	0.0343 (6)
N4	0.2298 (3)	0.24994 (14)	0.33969 (14)	0.0278 (5)
O1	0.7668 (3)	0.23374 (14)	0.65682 (13)	0.0428 (6)
O2	1.0259 (3)	0.26347 (13)	0.71064 (12)	0.0371 (5)
O3	1.4018 (3)	0.43829 (16)	0.56198 (14)	0.0511 (6)
O4	1.2972 (3)	0.48619 (14)	0.44202 (13)	0.0450 (6)
H4A	1.3920	0.5075	0.4448	0.068*
O5	0.7363 (3)	0.39334 (15)	0.30987 (12)	0.0443 (6)
O6	0.5753 (3)	0.31807 (13)	0.38107 (13)	0.0372 (5)
O1W	0.4422 (6)	0.2569 (4)	0.5980 (4)	0.1444 (18)
H1A	0.559 (4)	0.247 (5)	0.610 (6)	0.217*
H1B	0.436 (11)	0.3110 (17)	0.588 (6)	0.217*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0260 (2)	0.0274 (2)	0.0221 (2)	−0.00004 (16)	0.00142 (15)	0.00103 (15)
C1	0.0325 (15)	0.0245 (15)	0.0236 (14)	−0.0015 (11)	0.0038 (12)	0.0011 (11)
C2	0.0306 (15)	0.0314 (16)	0.0215 (14)	−0.0007 (12)	0.0004 (11)	0.0005 (11)

C3	0.0266 (14)	0.0291 (15)	0.0256 (15)	−0.0028 (11)	0.0041 (11)	−0.0011 (11)
C4	0.0309 (15)	0.0278 (15)	0.0218 (14)	−0.0019 (12)	0.0037 (11)	0.0037 (11)
C5	0.0279 (14)	0.0277 (15)	0.0225 (14)	−0.0027 (11)	0.0021 (11)	0.0004 (11)
C6	0.0294 (15)	0.0301 (16)	0.0243 (14)	−0.0047 (12)	0.0022 (12)	−0.0010 (11)
C7	0.0393 (17)	0.0258 (15)	0.0242 (15)	−0.0006 (12)	0.0073 (12)	0.0025 (11)
C8	0.0366 (16)	0.0341 (17)	0.0262 (15)	−0.0057 (13)	0.0056 (13)	−0.0011 (12)
C9	0.0306 (15)	0.0314 (16)	0.0243 (15)	−0.0008 (12)	−0.0010 (12)	−0.0018 (12)
C10	0.0276 (15)	0.0259 (15)	0.0364 (17)	−0.0063 (11)	0.0060 (12)	0.0002 (12)
C11	0.0348 (16)	0.0275 (16)	0.0331 (16)	−0.0043 (12)	0.0079 (13)	−0.0022 (12)
C12	0.0295 (15)	0.0317 (16)	0.0365 (17)	−0.0035 (12)	0.0089 (13)	0.0045 (13)
C13	0.0352 (16)	0.0417 (19)	0.0312 (17)	−0.0066 (14)	0.0051 (13)	0.0014 (13)
C14	0.0384 (17)	0.0385 (19)	0.0414 (19)	−0.0047 (14)	0.0115 (15)	−0.0089 (14)
C15	0.0282 (15)	0.0305 (16)	0.0434 (18)	−0.0009 (12)	0.0073 (13)	−0.0041 (13)
C16	0.0385 (17)	0.0290 (16)	0.0369 (17)	−0.0050 (13)	0.0045 (14)	0.0038 (13)
C17	0.0408 (18)	0.045 (2)	0.044 (2)	0.0059 (15)	0.0176 (15)	0.0125 (15)
C18	0.0359 (17)	0.0256 (16)	0.0373 (17)	0.0034 (12)	−0.0019 (13)	0.0000 (12)
C19	0.0400 (18)	0.0276 (17)	0.0373 (17)	0.0057 (13)	0.0032 (14)	−0.0014 (13)
C20	0.0348 (17)	0.0324 (17)	0.0388 (17)	0.0069 (13)	0.0036 (13)	−0.0017 (13)
C21	0.0261 (15)	0.0322 (16)	0.0362 (17)	0.0004 (12)	0.0033 (12)	0.0010 (13)
C22	0.0245 (15)	0.0405 (19)	0.0454 (19)	−0.0068 (13)	0.0017 (13)	0.0048 (14)
C23	0.0289 (16)	0.0371 (18)	0.0374 (17)	−0.0015 (13)	0.0002 (13)	0.0003 (13)
N1	0.0325 (13)	0.0291 (14)	0.0303 (13)	−0.0005 (10)	−0.0002 (10)	0.0002 (10)
N2	0.0329 (13)	0.0232 (13)	0.0313 (13)	−0.0001 (10)	0.0021 (10)	−0.0018 (10)
N3	0.0304 (13)	0.0325 (14)	0.0412 (16)	−0.0005 (11)	0.0088 (11)	0.0078 (11)
N4	0.0252 (12)	0.0279 (13)	0.0305 (13)	−0.0006 (10)	0.0037 (10)	0.0000 (10)
O1	0.0420 (13)	0.0486 (14)	0.0372 (13)	−0.0145 (11)	0.0020 (10)	0.0138 (10)
O2	0.0379 (12)	0.0453 (14)	0.0268 (11)	−0.0039 (10)	−0.0021 (9)	0.0091 (9)
O3	0.0370 (13)	0.0736 (18)	0.0401 (14)	−0.0219 (12)	−0.0072 (11)	0.0147 (12)
O4	0.0385 (12)	0.0586 (15)	0.0377 (13)	−0.0183 (11)	0.0027 (10)	0.0104 (11)
O5	0.0459 (13)	0.0598 (15)	0.0258 (12)	−0.0092 (11)	−0.0016 (10)	0.0140 (10)
O6	0.0311 (11)	0.0514 (14)	0.0279 (11)	−0.0125 (10)	−0.0025 (9)	0.0017 (9)
O1W	0.109 (3)	0.190 (5)	0.132 (4)	0.003 (4)	0.006 (3)	0.019 (4)

Geometric parameters (Å, °)

Co1—O6[i]	1.968 (2)	C14—C15	1.379 (4)
Co1—O2	2.024 (2)	C14—H14	0.9300
Co1—N1	2.026 (2)	C15—H15	0.9300
Co1—N4[i]	2.057 (2)	C16—N2	1.477 (4)
C1—C6	1.386 (4)	C16—H16A	0.9700
C1—C2	1.388 (4)	C16—H16B	0.9700
C1—C7	1.503 (4)	C17—N3	1.471 (4)
C2—C3	1.392 (4)	C17—H17A	0.9700
C2—H2	0.9300	C17—H17B	0.9700
C3—C4	1.395 (4)	C18—N1	1.318 (4)
C3—C8	1.490 (4)	C18—N2	1.333 (4)
C4—C5	1.390 (4)	C18—H18	0.9300
C4—H4	0.9300	C19—C20	1.345 (4)
C5—C6	1.390 (4)	C19—N2	1.371 (4)

C5—C9	1.508 (4)	C19—H19	0.9300
C6—H6	0.9300	C20—N1	1.378 (4)
C7—O1	1.250 (3)	C20—H20	0.9300
C7—O2	1.266 (4)	C21—N4	1.322 (4)
C8—O3	1.240 (4)	C21—N3	1.346 (4)
C8—O4	1.286 (3)	C21—H21	0.9300
C9—O5	1.228 (3)	C22—C23	1.356 (4)
C9—O6	1.277 (3)	C22—N3	1.366 (4)
C10—C11	1.390 (4)	C22—H22	0.9300
C10—C15	1.395 (4)	C23—N4	1.387 (4)
C10—C16	1.513 (4)	C23—H23	0.9300
C11—C12	1.389 (4)	N4—Co1^{ii}	2.057 (2)
C11—H11	0.9300	O4—H4A	0.8200
C12—C13	1.392 (4)	O6—Co1^{ii}	1.968 (2)
C12—C17	1.511 (4)	O1W—H1A	0.93 (2)
C13—C14	1.384 (4)	O1W—H1B	0.91 (2)
C13—H13	0.9300		
O6^{i}—Co1—O2	103.70 (9)	C14—C15—H15	119.7
O6^{i}—Co1—N1	111.27 (9)	C10—C15—H15	119.7
O2—Co1—N1	127.96 (9)	N2—C16—C10	111.0 (2)
O6^{i}—Co1—N4^{i}	94.21 (9)	N2—C16—H16A	109.4
O2—Co1—N4^{i}	110.41 (9)	C10—C16—H16A	109.4
N1—Co1—N4^{i}	104.23 (9)	N2—C16—H16B	109.4
C6—C1—C2	119.8 (3)	C10—C16—H16B	109.4
C6—C1—C7	119.7 (3)	H16A—C16—H16B	108.0
C2—C1—C7	120.4 (3)	N3—C17—C12	114.4 (3)
C1—C2—C3	119.5 (3)	N3—C17—H17A	108.7
C1—C2—H2	120.3	C12—C17—H17A	108.7
C3—C2—H2	120.3	N3—C17—H17B	108.7
C2—C3—C4	120.5 (3)	C12—C17—H17B	108.7
C2—C3—C8	119.4 (3)	H17A—C17—H17B	107.6
C4—C3—C8	120.1 (2)	N1—C18—N2	111.5 (3)
C5—C4—C3	120.0 (2)	N1—C18—H18	124.3
C5—C4—H4	120.0	N2—C18—H18	124.3
C3—C4—H4	120.0	C20—C19—N2	106.5 (3)
C4—C5—C6	119.0 (3)	C20—C19—H19	126.7
C4—C5—C9	120.5 (2)	N2—C19—H19	126.7
C6—C5—C9	120.4 (2)	C19—C20—N1	109.3 (3)
C1—C6—C5	121.2 (3)	C19—C20—H20	125.3
C1—C6—H6	119.4	N1—C20—H20	125.3
C5—C6—H6	119.4	N4—C21—N3	111.4 (3)
O1—C7—O2	120.9 (3)	N4—C21—H21	124.3
O1—C7—C1	120.5 (3)	N3—C21—H21	124.3
O2—C7—C1	118.7 (3)	C23—C22—N3	107.1 (3)
O3—C8—O4	123.8 (3)	C23—C22—H22	126.4
O3—C8—C3	120.7 (3)	N3—C22—H22	126.4
O4—C8—C3	115.5 (3)	C22—C23—N4	108.7 (3)

O5—C9—O6	124.1 (3)	C22—C23—H23	125.6
O5—C9—C5	120.7 (3)	N4—C23—H23	125.6
O6—C9—C5	115.2 (2)	C18—N1—C20	105.5 (2)
C11—C10—C15	118.5 (3)	C18—N1—Co1	122.7 (2)
C11—C10—C16	119.9 (3)	C20—N1—Co1	131.2 (2)
C15—C10—C16	121.5 (3)	C18—N2—C19	107.1 (2)
C12—C11—C10	121.2 (3)	C18—N2—C16	125.9 (2)
C12—C11—H11	119.4	C19—N2—C16	126.9 (2)
C10—C11—H11	119.4	C21—N3—C22	107.0 (3)
C11—C12—C13	119.3 (3)	C21—N3—C17	125.3 (3)
C11—C12—C17	116.9 (3)	C22—N3—C17	127.6 (3)
C13—C12—C17	123.8 (3)	C21—N4—C23	105.7 (2)
C14—C13—C12	119.8 (3)	C21—N4—Co1[ii]	122.36 (19)
C14—C13—H13	120.1	C23—N4—Co1[ii]	131.9 (2)
C12—C13—H13	120.1	C7—O2—Co1	99.08 (17)
C15—C14—C13	120.6 (3)	C8—O4—H4A	109.5
C15—C14—H14	119.7	C9—O6—Co1[ii]	114.27 (18)
C13—C14—H14	119.7	H1A—O1W—H1B	104 (4)
C14—C15—C10	120.5 (3)		
C6—C1—C2—C3	−0.1 (4)	C13—C12—C17—N3	−28.7 (4)
C7—C1—C2—C3	176.4 (3)	N2—C19—C20—N1	−0.2 (3)
C1—C2—C3—C4	0.4 (4)	N3—C22—C23—N4	−0.6 (4)
C1—C2—C3—C8	−178.1 (3)	N2—C18—N1—C20	0.3 (3)
C2—C3—C4—C5	−0.6 (4)	N2—C18—N1—Co1	−171.73 (18)
C8—C3—C4—C5	177.9 (3)	C19—C20—N1—C18	−0.1 (3)
C3—C4—C5—C6	0.6 (4)	C19—C20—N1—Co1	171.1 (2)
C3—C4—C5—C9	−178.4 (2)	O6[i]—Co1—N1—C18	130.6 (2)
C2—C1—C6—C5	0.1 (4)	O2—Co1—N1—C18	−100.6 (2)
C7—C1—C6—C5	−176.4 (3)	N4[i]—Co1—N1—C18	30.3 (3)
C4—C5—C6—C1	−0.3 (4)	O6[i]—Co1—N1—C20	−39.2 (3)
C9—C5—C6—C1	178.7 (3)	O2—Co1—N1—C20	89.6 (3)
C6—C1—C7—O1	−5.4 (4)	N4[i]—Co1—N1—C20	−139.6 (3)
C2—C1—C7—O1	178.1 (3)	N1—C18—N2—C19	−0.5 (3)
C6—C1—C7—O2	172.9 (3)	N1—C18—N2—C16	−178.5 (3)
C2—C1—C7—O2	−3.7 (4)	C20—C19—N2—C18	0.4 (3)
C2—C3—C8—O3	5.2 (4)	C20—C19—N2—C16	178.4 (3)
C4—C3—C8—O3	−173.4 (3)	C10—C16—N2—C18	69.2 (4)
C2—C3—C8—O4	−174.8 (3)	C10—C16—N2—C19	−108.5 (3)
C4—C3—C8—O4	6.6 (4)	N4—C21—N3—C22	−1.1 (3)
C4—C5—C9—O5	0.4 (4)	N4—C21—N3—C17	−179.2 (3)
C6—C5—C9—O5	−178.6 (3)	C23—C22—N3—C21	1.0 (4)
C4—C5—C9—O6	−179.9 (3)	C23—C22—N3—C17	179.0 (3)
C6—C5—C9—O6	1.1 (4)	C12—C17—N3—C21	−80.6 (4)
C15—C10—C11—C12	−1.6 (4)	C12—C17—N3—C22	101.7 (4)
C16—C10—C11—C12	177.8 (3)	N3—C21—N4—C23	0.8 (3)
C10—C11—C12—C13	1.4 (4)	N3—C21—N4—Co1[ii]	−177.61 (19)
C10—C11—C12—C17	179.8 (3)	C22—C23—N4—C21	−0.1 (3)

C11—C12—C13—C14	−0.9 (4)	C22—C23—N4—Co1[ii]	178.1 (2)
C17—C12—C13—C14	−179.2 (3)	O1—C7—O2—Co1	0.7 (3)
C12—C13—C14—C15	0.6 (4)	C1—C7—O2—Co1	−177.5 (2)
C13—C14—C15—C10	−0.8 (4)	O6[i]—Co1—O2—C7	−174.51 (17)
C11—C10—C15—C14	1.3 (4)	N1—Co1—O2—C7	53.9 (2)
C16—C10—C15—C14	−178.1 (3)	N4[i]—Co1—O2—C7	−74.65 (19)
C11—C10—C16—N2	−87.8 (3)	O5—C9—O6—Co1[ii]	2.9 (4)
C15—C10—C16—N2	91.4 (3)	C5—C9—O6—Co1[ii]	−176.79 (18)
C11—C12—C17—N3	152.9 (3)		

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

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1A···O1	0.93 (2)	1.74 (3)	2.657 (5)	166 (9)
O4—H4A···O3[iii]	0.82	1.87	2.680 (3)	173

Symmetry codes: (iii) $-x+3$, $-y+1$, $-z+1$.

Fig. 1

Fig. 2

Fig. 3