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(5,5′-Dicarboxybiphenyl-2,2′-dicarboxylato-$\kappa^2O^2,O^{2'}$)bis(1,10-phenanthroline-κ^2N,N')cobalt(II) dihydrate

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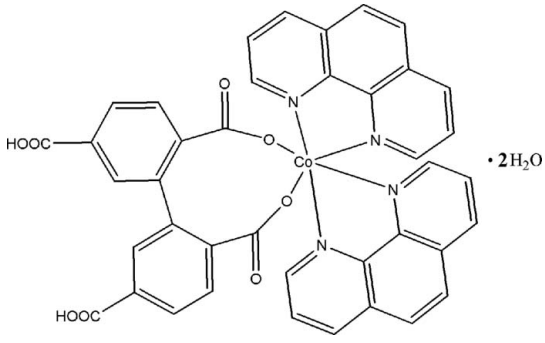
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.048; wR factor = 0.111; data-to-parameter ratio = 13.5.

In the title compound, $[Co(C_{16}H_8O_8)(C_{12}H_8N_2)_2]\cdot 2H_2O$, the Co atom located on a twofold rotation axis. It is six-coordinated by two O atoms from one 5,5′-dicarboxybiphenyl-2,2′-dicarboxylate anion and four N atoms from two 1,10-phenanthroline molecules in a distorted octahedral environment. The crystal packing is stabilized by O—H···O hydrogen bonds.

Related literature

For related literature, see: Zang *et al.* (2006); Che *et al.* (2006); Lehn (1990).



Experimental

Crystal data

$[Co(C_{16}H_8O_8)(C_{12}H_8N_2)_2]\cdot 2H_2O$
M_r = 783.59
Monoclinic, $C2/c$
a = 16.9272 (14) Å
b = 9.4514 (8) Å
c = 22.0458 (19) Å
β = 96.056 (1)°
V = 3507.3 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.56 mm^{-1}
T = 293 (2) K
0.28 × 0.25 × 0.23 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.852, T_{max} = 0.880
9540 measured reflections
3447 independent reflections
2705 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.111
S = 1.05
3447 reflections
255 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Selected bond lengths (Å).

N1—Co1	2.121 (2)	O1—Co1	2.0865 (16)
N2—Co1	2.155 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1A···O2	0.890 (10)	1.929 (11)	2.811 (3)	171 (3)
O4—H4···O2^{i}	0.82	1.74	2.535 (2)	163
O1W—H1B···O3^{ii}	0.889 (10)	2.177 (19)	2.934 (3)	143 (2)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2694).

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supporting information

Acta Cryst. (2008). E**64**, m761 [doi:10.1107/S160053680801012X]

(5,5′-Dicarboxybiphenyl-2,2′-dicarboxylato-$\kappa^2O^2,O^{2'}$)bis(1,10-phenanthroline-κ^2N,N')cobalt(II) dihydrate

Ruizhan Chen, Feijun Guo and Fanlei Meng

S1. Comment

Aromatic polycarboxylate ligands have been extensively employed in the preparation of metal-organic coordination complexes due to their ability to form networks and due to their interesting properties (Lehn, 1990; Che *et al.*, 2006). We selected biphenyl-2,5,2′,5′-tetracarboxylic acid (H_4BPTC) as a bridging ligand, 1,10-phenanthroline as a neutral ligand, and Co^{II} as a metal center, in order to generate a new compound, $[Co(H_2BPTC)(Phen)_2]\cdot 2H_2O$, (I), which is reported here.

In compound (I), each Co^{II} atom is six-coordinated by two O atoms from one H_2BPTC anion and four N atoms from two 1,10-phenanthroline molecules in a distorted octahedral environment (Fig. 1). The bond lengths are all within the normal ranges (Zang *et al.*, 2006). The crystal packing is stabilized by O—H···O hydrogen bonds between carboxylate groups and water molecules.

S2. Experimental

A mixture of $CoCl_2\cdot 2H_2O$ (0.1 mmol), biphenyl-2,5,2′,5′-tetracarboxylic acid (0.2 mmol), 1,10-phenanthroline (0.2 mmol) and H_2O(15 ml) in a 25 ml stainless steel reactor with a Teflon liner was heated from 298 to 443 K in 2 h and a constant temperature was maintained at 443 K for 72 h, after which the mixture was cooled to 298 K. Then, pink crystals of were obtained.

S3. Refinement

The water H-atoms were located from a difference Fourier map, and were refined with distance restraints of O–H = 0.90 Å and U_{iso}(H) = 1.5U_{eq}(O). Other H atoms were positioned geometrically (C—H = 0.93 Å and O—H = 0.82 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) and U_{iso}(H) = 1.5U_{eq}(O).

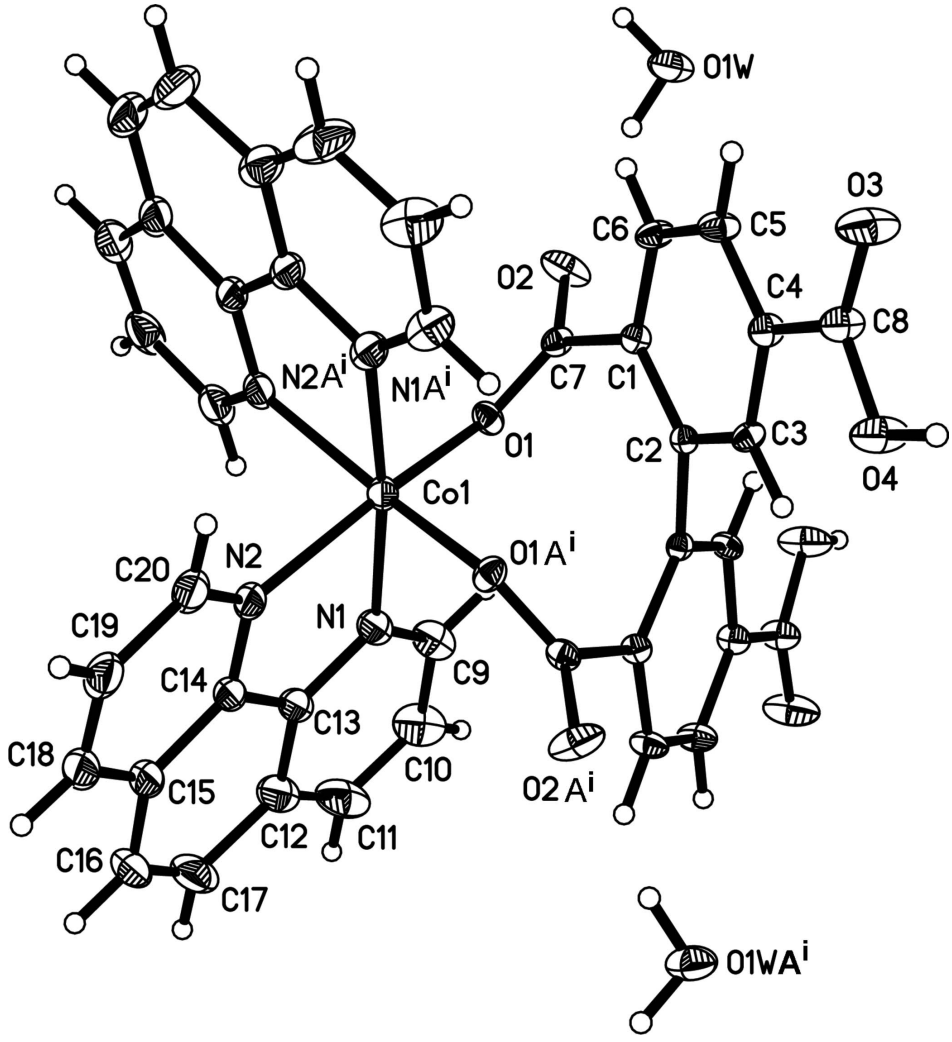

Figure 1

The structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Symmetry code: (i) -*x*, *y*, 0.5 - *z*.

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c = 22.0458 (19) Å
β = 96.056 (1)°
V = 3507.3 (5) Å^3
Z = 4
F(000) = 1612
D_x = 1.484 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 3447 reflections
θ = 2.0–26.0°
μ = 0.56 mm^{-1}
T = 293 K
Block, pink
0.28 × 0.25 × 0.23 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.852, T_{max} = 0.880
9540 measured reflections
3447 independent reflections
2705 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 26.0°, θ_{min} = 1.9°
h = −20→20
k = −11→10
l = −27→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.111
S = 1.05
3447 reflections
255 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0514P)^2 + 0.7022P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	0.02180 (12)	0.3926 (2)	0.17029 (10)	0.0195 (5)
C2	−0.01759 (12)	0.4503 (2)	0.21744 (10)	0.0176 (5)
C3	−0.08951 (13)	0.5192 (2)	0.20193 (10)	0.0210 (5)
H3	−0.1170	0.5561	0.2327	0.025*
C4	−0.12130 (13)	0.5340 (3)	0.14147 (11)	0.0240 (5)
C5	−0.07984 (13)	0.4819 (3)	0.09534 (11)	0.0281 (6)
H5	−0.0999	0.4935	0.0547	0.034*
C6	−0.00843 (13)	0.4127 (3)	0.11002 (11)	0.0265 (6)
H6	0.0197	0.3791	0.0790	0.032*
C7	0.09258 (13)	0.2983 (2)	0.18419 (11)	0.0227 (5)
C8	−0.19930 (14)	0.6078 (3)	0.12529 (11)	0.0305 (6)
C9	0.12655 (16)	0.1382 (3)	0.36037 (13)	0.0419 (7)
H9	0.1462	0.2070	0.3358	0.050*
C10	0.16476 (18)	0.1183 (4)	0.41931 (15)	0.0551 (9)
H10	0.2081	0.1740	0.4335	0.066*

C11	0.13745 (19)	0.0158 (4)	0.45565 (15)	0.0579 (10)
H11	0.1632	−0.0008	0.4944	0.069*
C12	0.07085 (19)	−0.0637 (3)	0.43443 (14)	0.0463 (8)
C13	0.03635 (17)	−0.0368 (3)	0.37519 (13)	0.0369 (7)
C14	−0.03385 (18)	−0.1126 (3)	0.35129 (13)	0.0393 (7)
C15	−0.0675 (2)	−0.2122 (3)	0.38854 (15)	0.0500 (8)
C16	−0.0295 (3)	−0.2393 (4)	0.44813 (17)	0.0651 (11)
H16	−0.0508	−0.3072	0.4723	0.078*
C17	0.0364 (2)	−0.1692 (4)	0.47042 (16)	0.0637 (10)
H17	0.0598	−0.1893	0.5095	0.076*
C18	−0.1378 (2)	−0.2783 (3)	0.36436 (17)	0.0612 (10)
H18	−0.1619	−0.3455	0.3871	0.073*
C19	−0.1707 (2)	−0.2438 (3)	0.30749 (17)	0.0573 (10)
H19	−0.2184	−0.2849	0.2915	0.069*
C20	−0.13227 (18)	−0.1458 (3)	0.27306 (15)	0.0472 (8)
H20	−0.1551	−0.1239	0.2339	0.057*
N1	0.06377 (12)	0.0635 (2)	0.33797 (10)	0.0342 (5)
N2	−0.06511 (14)	−0.0830 (2)	0.29367 (11)	0.0369 (6)
O1	0.09051 (9)	0.20921 (16)	0.22641 (7)	0.0257 (4)
O2	0.14953 (10)	0.3116 (2)	0.15270 (8)	0.0443 (5)
O1W	0.16597 (12)	0.4484 (2)	0.04153 (9)	0.0432 (5)
O3	−0.22748 (11)	0.6294 (2)	0.07347 (8)	0.0507 (6)
O4	−0.23287 (10)	0.6461 (2)	0.17334 (8)	0.0475 (6)
H4	−0.2751	0.6858	0.1626	0.071*
Co1	0.0000	0.07672 (5)	0.2500	0.02804 (17)
H1A	0.1647 (16)	0.398 (3)	0.0755 (8)	0.042*
H1B	0.1857 (15)	0.388 (2)	0.0163 (10)	0.042*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0143 (10)	0.0227 (13)	0.0218 (12)	0.0028 (9)	0.0030 (9)	0.0004 (10)
C2	0.0153 (11)	0.0177 (12)	0.0199 (12)	−0.0020 (9)	0.0029 (9)	0.0005 (9)
C3	0.0181 (11)	0.0248 (13)	0.0203 (13)	0.0026 (9)	0.0033 (10)	−0.0037 (10)
C4	0.0193 (12)	0.0288 (14)	0.0238 (13)	0.0063 (10)	0.0016 (10)	0.0001 (10)
C5	0.0236 (12)	0.0418 (16)	0.0180 (13)	0.0087 (11)	−0.0021 (10)	0.0010 (11)
C6	0.0245 (12)	0.0360 (15)	0.0196 (13)	0.0085 (11)	0.0058 (10)	−0.0030 (11)
C7	0.0198 (12)	0.0260 (13)	0.0222 (13)	0.0052 (10)	0.0019 (10)	−0.0028 (10)
C8	0.0227 (12)	0.0443 (17)	0.0242 (14)	0.0110 (11)	0.0020 (11)	0.0005 (12)
C9	0.0319 (15)	0.0500 (18)	0.0444 (18)	0.0084 (14)	0.0072 (13)	0.0125 (14)
C10	0.0368 (16)	0.079 (3)	0.048 (2)	0.0138 (16)	−0.0001 (15)	0.0097 (18)
C11	0.051 (2)	0.081 (3)	0.0416 (19)	0.0279 (19)	0.0070 (16)	0.0244 (18)
C12	0.0533 (19)	0.0457 (19)	0.0425 (18)	0.0193 (15)	0.0168 (15)	0.0117 (15)
C13	0.0483 (17)	0.0286 (15)	0.0371 (17)	0.0160 (13)	0.0195 (14)	0.0069 (12)
C14	0.0587 (19)	0.0238 (15)	0.0404 (17)	0.0087 (13)	0.0283 (15)	0.0025 (12)
C15	0.079 (2)	0.0265 (16)	0.051 (2)	0.0043 (16)	0.0385 (18)	0.0022 (14)
C16	0.106 (3)	0.038 (2)	0.060 (2)	0.007 (2)	0.048 (2)	0.0151 (17)
C17	0.092 (3)	0.055 (2)	0.049 (2)	0.026 (2)	0.029 (2)	0.0256 (18)

C18	0.094 (3)	0.0323 (18)	0.067 (3)	−0.0128 (18)	0.056 (2)	−0.0067 (16)
C19	0.074 (2)	0.0376 (18)	0.068 (2)	−0.0217 (17)	0.043 (2)	−0.0196 (17)
C20	0.060 (2)	0.0317 (16)	0.054 (2)	−0.0110 (15)	0.0279 (16)	−0.0119 (14)
N1	0.0352 (12)	0.0323 (13)	0.0367 (13)	0.0091 (10)	0.0119 (10)	0.0061 (10)
N2	0.0485 (14)	0.0236 (12)	0.0426 (14)	−0.0036 (11)	0.0238 (12)	−0.0048 (10)
O1	0.0231 (9)	0.0249 (9)	0.0294 (10)	0.0044 (7)	0.0038 (7)	0.0069 (8)
O2	0.0297 (10)	0.0664 (14)	0.0402 (12)	0.0286 (9)	0.0196 (9)	0.0277 (10)
O1W	0.0472 (12)	0.0570 (14)	0.0262 (11)	0.0127 (10)	0.0079 (9)	0.0085 (9)
O3	0.0378 (11)	0.0889 (17)	0.0242 (11)	0.0349 (11)	−0.0027 (9)	0.0028 (10)
O4	0.0356 (11)	0.0810 (15)	0.0264 (10)	0.0384 (10)	0.0057 (9)	0.0074 (10)
Co1	0.0308 (3)	0.0225 (3)	0.0323 (3)	0.000	0.0103 (2)	0.000

Geometric parameters (Å, º)

C1—C6	1.385 (3)	C13—N1	1.367 (3)
C1—C2	1.403 (3)	C13—C14	1.439 (4)
C1—C7	1.499 (3)	C14—N2	1.353 (4)
C2—C3	1.391 (3)	C14—C15	1.408 (4)
C2—C2^{i}	1.495 (4)	C15—C18	1.399 (5)
C3—C4	1.391 (3)	C15—C16	1.424 (5)
C3—H3	0.9300	C16—C17	1.345 (5)
C4—C5	1.385 (3)	C16—H16	0.9300
C4—C8	1.503 (3)	C17—H17	0.9300
C5—C6	1.382 (3)	C18—C19	1.357 (5)
C5—H5	0.9300	C18—H18	0.9300
C6—H6	0.9300	C19—C20	1.401 (4)
C7—O2	1.252 (3)	C19—H19	0.9300
C7—O1	1.258 (3)	C20—N2	1.320 (4)
C8—O3	1.208 (3)	C20—H20	0.9300
C8—O4	1.305 (3)	N1—Co1	2.121 (2)
C9—N1	1.327 (3)	N2—Co1	2.155 (2)
C9—C10	1.402 (4)	O1—Co1	2.0865 (16)
C9—H9	0.9300	O1W—H1A	0.890 (10)
C10—C11	1.368 (4)	O1W—H1B	0.889 (10)
C10—H10	0.9300	O4—H4	0.8200
C11—C12	1.394 (5)	Co1—O1^{i}	2.0865 (16)
C11—H11	0.9300	Co1—N1^{i}	2.121 (2)
C12—C13	1.396 (4)	Co1—N2^{i}	2.155 (2)
C12—C17	1.437 (4)		
C6—C1—C2	120.1 (2)	C18—C15—C14	117.2 (3)
C6—C1—C7	118.9 (2)	C18—C15—C16	123.7 (3)
C2—C1—C7	120.8 (2)	C14—C15—C16	119.2 (3)
C3—C2—C1	118.1 (2)	C17—C16—C15	121.7 (3)
C3—C2—C2^{i}	119.1 (2)	C17—C16—H16	119.2
C1—C2—C2^{i}	122.6 (2)	C15—C16—H16	119.2
C2—C3—C4	121.5 (2)	C16—C17—C12	120.7 (3)
C2—C3—H3	119.2	C16—C17—H17	119.7

C4—C3—H3	119.2	C12—C17—H17	119.7
C5—C4—C3	119.5 (2)	C19—C18—C15	119.6 (3)
C5—C4—C8	119.4 (2)	C19—C18—H18	120.2
C3—C4—C8	121.0 (2)	C15—C18—H18	120.2
C6—C5—C4	119.6 (2)	C18—C19—C20	119.4 (3)
C6—C5—H5	120.2	C18—C19—H19	120.3
C4—C5—H5	120.2	C20—C19—H19	120.3
C5—C6—C1	121.0 (2)	N2—C20—C19	122.9 (3)
C5—C6—H6	119.5	N2—C20—H20	118.5
C1—C6—H6	119.5	C19—C20—H20	118.5
O2—C7—O1	124.1 (2)	C9—N1—C13	117.1 (2)
O2—C7—C1	118.2 (2)	C9—N1—Co1	128.26 (19)
O1—C7—C1	117.7 (2)	C13—N1—Co1	114.67 (19)
O3—C8—O4	124.0 (2)	C20—N2—C14	117.9 (3)
O3—C8—C4	123.5 (2)	C20—N2—Co1	128.6 (2)
O4—C8—C4	112.5 (2)	C14—N2—Co1	113.37 (18)
N1—C9—C10	123.2 (3)	C7—O1—Co1	131.64 (15)
N1—C9—H9	118.4	H1A—O1W—H1B	103 (3)
C10—C9—H9	118.4	C8—O4—H4	109.5
C11—C10—C9	119.1 (3)	O1—Co1—O1^{i}	106.24 (9)
C11—C10—H10	120.5	O1—Co1—N1^{i}	97.10 (7)
C9—C10—H10	120.5	O1^{i}—Co1—N1^{i}	86.97 (7)
C10—C11—C12	119.8 (3)	O1—Co1—N1	86.97 (7)
C10—C11—H11	120.1	O1^{i}—Co1—N1	97.10 (7)
C12—C11—H11	120.1	N1^{i}—Co1—N1	173.25 (12)
C11—C12—C13	117.4 (3)	O1—Co1—N2	162.80 (8)
C11—C12—C17	123.4 (3)	O1^{i}—Co1—N2	83.42 (7)
C13—C12—C17	119.2 (3)	N1^{i}—Co1—N2	97.60 (9)
N1—C13—C12	123.5 (3)	N1—Co1—N2	77.60 (9)
N1—C13—C14	116.4 (3)	O1—Co1—N2^{i}	83.42 (7)
C12—C13—C14	120.0 (3)	O1^{i}—Co1—N2^{i}	162.80 (8)
N2—C14—C15	122.9 (3)	N1^{i}—Co1—N2^{i}	77.60 (9)
N2—C14—C13	117.8 (2)	N1—Co1—N2^{i}	97.60 (8)
C15—C14—C13	119.2 (3)	N2—Co1—N2^{i}	91.07 (11)

C6—C1—C2—C3	4.1 (3)	C14—C15—C18—C19	−0.7 (4)
C7—C1—C2—C3	−170.5 (2)	C16—C15—C18—C19	178.7 (3)
C6—C1—C2—C2^{i}	−171.09 (18)	C15—C18—C19—C20	2.1 (5)
C7—C1—C2—C2^{i}	14.4 (3)	C18—C19—C20—N2	−0.8 (5)
C1—C2—C3—C4	−1.4 (3)	C10—C9—N1—C13	0.0 (4)
C2^{i}—C2—C3—C4	173.90 (19)	C10—C9—N1—Co1	−178.9 (2)
C2—C3—C4—C5	−1.4 (4)	C12—C13—N1—C9	0.0 (4)
C2—C3—C4—C8	179.6 (2)	C14—C13—N1—C9	177.3 (2)
C3—C4—C5—C6	1.7 (4)	C12—C13—N1—Co1	179.0 (2)
C8—C4—C5—C6	−179.4 (2)	C14—C13—N1—Co1	−3.6 (3)
C4—C5—C6—C1	1.0 (4)	C19—C20—N2—C14	−1.9 (4)
C2—C1—C6—C5	−3.9 (4)	C19—C20—N2—Co1	−176.8 (2)
C7—C1—C6—C5	170.7 (2)	C15—C14—N2—C20	3.4 (4)

C6—C1—C7—O2	45.0 (3)	C13—C14—N2—C20	−175.8 (2)
C2—C1—C7—O2	−140.4 (2)	C15—C14—N2—Co1	179.0 (2)
C6—C1—C7—O1	−134.1 (2)	C13—C14—N2—Co1	−0.1 (3)
C2—C1—C7—O1	40.5 (3)	O2—C7—O1—Co1	−137.2 (2)
C5—C4—C8—O3	−2.7 (4)	C1—C7—O1—Co1	41.8 (3)
C3—C4—C8—O3	176.3 (3)	C7—O1—Co1—O1^{i}	−63.12 (19)
C5—C4—C8—O4	177.5 (2)	C7—O1—Co1—N1^{i}	25.8 (2)
C3—C4—C8—O4	−3.6 (3)	C7—O1—Co1—N1	−159.6 (2)
N1—C9—C10—C11	1.1 (5)	C7—O1—Co1—N2	174.4 (2)
C9—C10—C11—C12	−2.1 (5)	C7—O1—Co1—N2^{i}	102.3 (2)
C10—C11—C12—C13	2.0 (4)	C9—N1—Co1—O1	9.2 (2)
C10—C11—C12—C17	−177.4 (3)	C13—N1—Co1—O1	−169.69 (17)
C11—C12—C13—N1	−0.9 (4)	C9—N1—Co1—O1^{i}	−96.8 (2)
C17—C12—C13—N1	178.5 (3)	C13—N1—Co1—O1^{i}	84.31 (17)
C11—C12—C13—C14	−178.3 (2)	C9—N1—Co1—N2	−178.4 (2)
C17—C12—C13—C14	1.2 (4)	C13—N1—Co1—N2	2.68 (17)
N1—C13—C14—N2	2.5 (3)	C9—N1—Co1—N2^{i}	92.2 (2)
C12—C13—C14—N2	180.0 (2)	C13—N1—Co1—N2^{i}	−86.74 (17)
N1—C13—C14—C15	−176.7 (2)	C20—N2—Co1—O1	−159.6 (2)
C12—C13—C14—C15	0.8 (4)	C14—N2—Co1—O1	25.3 (3)
N2—C14—C15—C18	−2.1 (4)	C20—N2—Co1—O1^{i}	75.0 (2)
C13—C14—C15—C18	177.0 (2)	C14—N2—Co1—O1^{i}	−100.13 (17)
N2—C14—C15—C16	178.4 (3)	C20—N2—Co1—N1^{i}	−11.1 (2)
C13—C14—C15—C16	−2.4 (4)	C14—N2—Co1—N1^{i}	173.83 (17)
C18—C15—C16—C17	−177.4 (3)	C20—N2—Co1—N1	173.8 (2)
C14—C15—C16—C17	2.1 (5)	C14—N2—Co1—N1	−1.35 (17)
C15—C16—C17—C12	0.0 (5)	C20—N2—Co1—N2^{i}	−88.7 (2)
C11—C12—C17—C16	177.8 (3)	C14—N2—Co1—N2^{i}	96.20 (19)
C13—C12—C17—C16	−1.6 (5)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*A*···O2	0.89 (1)	1.93 (1)	2.811 (3)	171 (3)
O4—H4···O2^{ii}	0.82	1.74	2.535 (2)	163
O1*W*—H1*B*···O3^{iii}	0.89 (1)	2.18 (2)	2.934 (3)	143 (2)

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