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catena-Poly[[(2,2′-bipyridine-κ^2N,N')-cobalt(II)]-μ-oxalato-$\kappa^4O^1,O^2:O^{1'},O^{2'}$]

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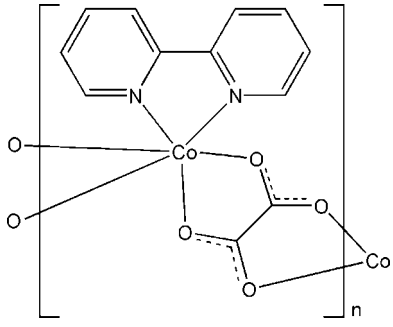
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.011 Å; R factor = 0.052; wR factor = 0.136; data-to-parameter ratio = 15.7.

In the one-dimensional title coordination polymer, $[Co(C_2O_4)(C_{10}H_8N_2)]_n$, the Co^{II} atom is coordinated in a distorted octahedral geometry by two N atoms from one 2,2′-bipyridine ligand and four O atoms belonging to two chelating oxalate ligands. Two neighboring Co centers are bridged by an oxalate ligand, forming a one-dimensional chain structure.

Related literature

For general background to metal–oxalate compounds, see: Coronado *et al.* (2001); Decurtins *et al.* (1994). For related structures, see: Fun *et al.* (1999); Lin *et al.* (2006).



Experimental

Crystal data

$[Co(C_2O_4)(C_{10}H_8N_2)]$
M_r = 303.13
Orthorhombic, $Pna2_1$
a = 9.2333 (18) Å
b = 9.2163 (18) Å
c = 14.101 (3) Å
V = 1199.9 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.44 mm^{-1}
T = 293 K
0.16 × 0.14 × 0.08 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.800, T_{max} = 0.892
10848 measured reflections
2692 independent reflections
1887 reflections with $I > 2\sigma(I)$
R_{int} = 0.064

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.136
S = 1.09
2692 reflections
172 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.90 e Å^{-3}
Absolute structure: Flack (1983); 1283 Friedel pairs
Flack parameter: 0.03 (4)

Table 1
Selected bond lengths (Å).

Co1—O1	2.076 (4)	Co1—N2	2.139 (5)
Co1—O4^{i}	2.095 (4)	Co1—O3	2.142 (4)
Co1—O2^{i}	2.126 (4)	Co1—N1	2.146 (5)

Symmetry code: (i) $x-\frac{1}{2}, -y+\frac{5}{2}, z$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *publCIF* (Westrip, 2009).

We thank AIST and Kobe University for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2191).

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supporting information

Acta Cryst. (2009). E**65**, m508 [doi:10.1107/S1600536809012690]

catena-Poly[[(2,2′-bipyridine-κ^2N,N')cobalt(II)]-μ-oxalato-$\kappa^4O^1,O^2:O^{1'},O^{2'}$]

Pei-Zhou Li and Qiang Xu

S1. Comment

The self-assembly of coordination polymers has attracted considerable attention in the past decade. This arises mainly for their various intriguing topological structures and their potential applications in material chemistry. Much research has been carried out on metal–oxalate compounds due to their interesting magnetic and optical properties (Coronado *et al.*, 2001; Decurtins *et al.*, 1994). Herein, we present the structure of the title complex, $[Co(C_2O_4)(C_{10}H_8N_2)]_n$, which is isomorphous to the zinc(II) complex reported by Lin *et al.* (2006) and to the iron(II) complex reported by Fun *et al.* (1999).

The title compound is an infinite one-dimensional coordination polymer. The Co^{II} atom is coordinated by two N atoms from one 2,2′-bipyridine ligand and four O atoms that belong to two oxalate dianions (Table 1) in a distorted octahedral geometry, as shown in Fig. 1. Two neighboring Co centers are bridged by an oxalate ligand, forming a one-dimensional chain structure, as shown in Fig. 2.

S2. Experimental

The brown plate-like single crystals of the title compound were obtained by a solvothermal reaction of cobalt chloride hexahydrate ($CoCl_2.6H_2O$, 0.5 mmol), sodium oxalate [$Na_2(C_2O_4)$, 1 mmol] and 2,2′-bipyridine ($C_{10}H_8N_2$, 0.5 mmol) in a solution of CH_3OH and H_2O (8 ml, volume ratio, 1:1) at 423 K for 24 h.

S3. Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

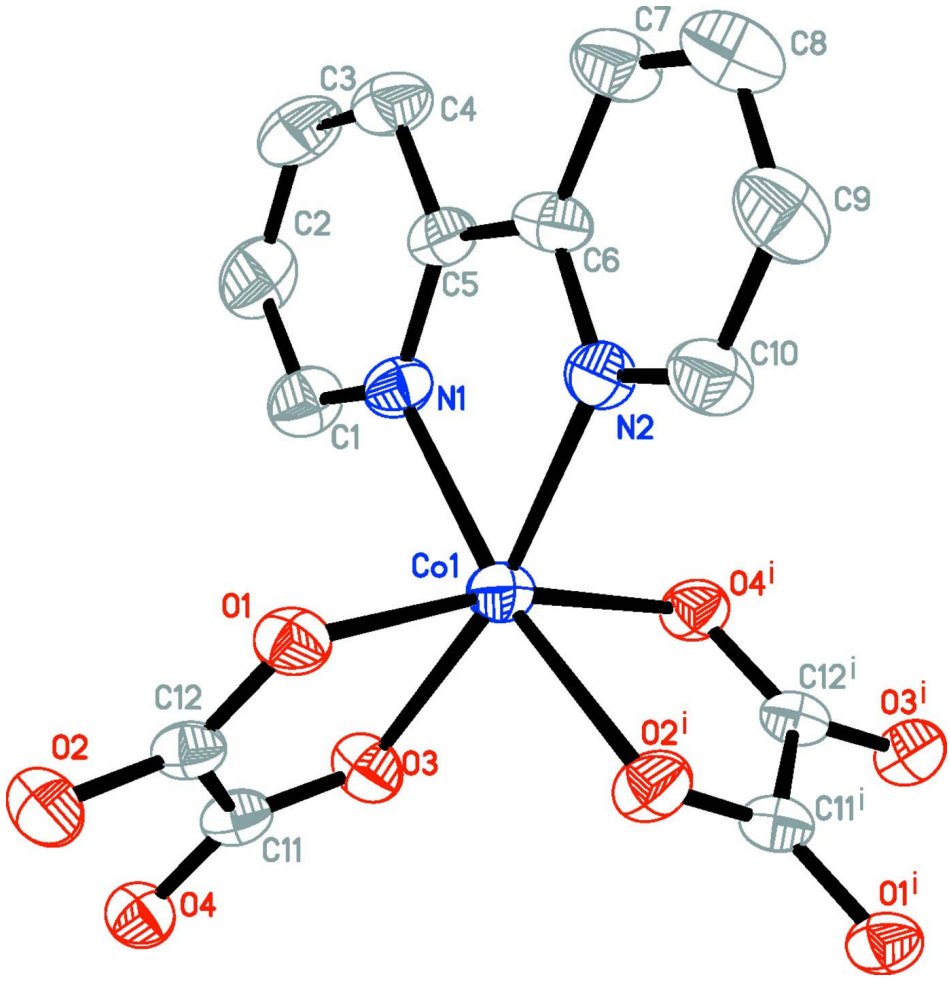

Figure 1

The asymmetric unit of the title compound, extended to show the Co coordination. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. [Symmetry code: (i) x-1/2, -y+5/2, z.]

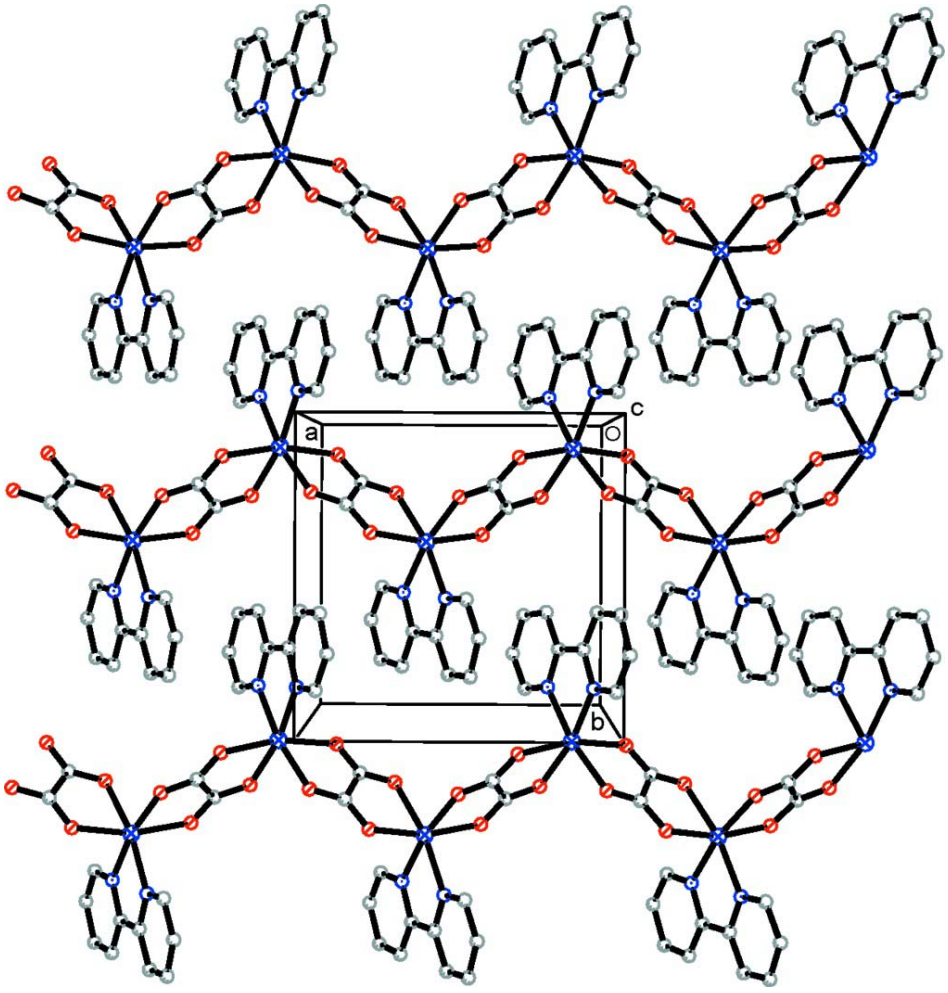

Figure 2

The one-dimensional chian structure of the title compound.

***catena*-Poly[[(2,2′-bipyridine-κ^2N,N')cobalt(II)]-μ-oxalato-$\kappa^4O^1,O^2:O^{1'},O^{2'}$]**

Crystal data

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Hall symbol: P 2c -2n
$a = 9.2333$ (18) Å
$b = 9.2163$ (18) Å
$c = 14.101$ (3) Å
$V = 1199.9$ (4) Å^3
$Z = 4$
$F(000) = 612$
$D_x = 1.678$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2143 reflections
$\theta = 3.4$–26.5°
$\mu = 1.44$ mm^{-1}
$T = 293$ K
Plate, brown
0.16 × 0.14 × 0.08 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: rotating anode
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.800$, $T_{max} = 0.892$
10848 measured reflections
2692 independent reflections

1887 reflections with $I > 2\sigma(I)$
$R_{int} = 0.064$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -10 \rightarrow 11$
$k = -11 \rightarrow 11$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.136$
$S = 1.09$
2692 reflections
172 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0501P)^2 + 1.1682P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.90$ e Å^{-3}
Absolute structure: Flack (1983); 1283 Friedel pairs
Absolute structure parameter: 0.03 (4)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O2	0.5044 (5)	1.2574 (5)	0.3939 (3)	0.0580 (13)
O4	0.4266 (4)	1.3874 (4)	0.2309 (3)	0.0507 (10)
C12	0.3425 (7)	1.2932 (7)	0.2640 (4)	0.0463 (14)
Co1	0.11792 (7)	1.08924 (7)	0.30925 (11)	0.0484 (2)
C11	0.3876 (6)	1.2177 (7)	0.3569 (4)	0.0441 (13)
O1	0.3038 (5)	1.1224 (4)	0.3891 (3)	0.0504 (10)
O3	0.2237 (5)	1.2560 (5)	0.2294 (3)	0.0543 (12)
C5	0.1633 (8)	0.7791 (7)	0.2550 (5)	0.0494 (15)
C6	0.0832 (8)	0.7718 (7)	0.3458 (5)	0.0519 (16)
N1	0.1983 (6)	0.9123 (6)	0.2254 (4)	0.0482 (12)
N2	0.0502 (6)	0.9010 (5)	0.3861 (4)	0.0485 (12)
C1	0.2749 (8)	0.9265 (8)	0.1462 (5)	0.0628 (18)
H1	0.3012	1.0189	0.1262	0.075*
C10	−0.0191 (8)	0.9026 (8)	0.4686 (5)	0.0630 (17)
H10	−0.0402	0.9916	0.4964	0.076*
C4	0.2031 (9)	0.6552 (8)	0.2047 (6)	0.066 (2)
H4	0.1776	0.5634	0.2264	0.079*
C9	−0.0611 (9)	0.7770 (9)	0.5146 (5)	0.074 (2)
H9	−0.1083	0.7819	0.5728	0.088*
C7	0.0401 (9)	0.6451 (8)	0.3887 (6)	0.069 (2)
H7	0.0604	0.5569	0.3596	0.083*
C2	0.3166 (9)	0.8083 (11)	0.0928 (6)	0.078 (2)
H2	0.3686	0.8209	0.0369	0.094*
C8	−0.0327 (10)	0.6461 (9)	0.4741 (6)	0.078 (2)
H8	−0.0615	0.5601	0.5031	0.094*
C3	0.2799 (10)	0.6717 (9)	0.1236 (6)	0.080 (2)
H3	0.3077	0.5907	0.0888	0.096*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.058 (3)	0.056 (3)	0.060 (3)	−0.010 (2)	−0.018 (3)	0.017 (2)
O4	0.057 (2)	0.046 (2)	0.049 (2)	−0.0021 (19)	−0.005 (2)	0.0123 (19)
C12	0.059 (3)	0.035 (3)	0.045 (3)	0.008 (3)	−0.003 (3)	0.002 (3)
Co1	0.0518 (4)	0.0394 (3)	0.0541 (4)	0.0005 (4)	−0.0009 (5)	−0.0032 (5)
C11	0.058 (4)	0.034 (3)	0.040 (3)	0.004 (3)	−0.007 (3)	0.001 (2)
O1	0.060 (2)	0.043 (2)	0.048 (2)	−0.0009 (19)	−0.007 (2)	0.0121 (19)
O3	0.058 (3)	0.055 (3)	0.050 (3)	−0.009 (2)	−0.014 (2)	0.009 (2)
C5	0.054 (3)	0.040 (3)	0.054 (4)	0.007 (3)	−0.004 (4)	0.000 (3)
C6	0.066 (4)	0.038 (3)	0.052 (4)	−0.007 (3)	−0.015 (4)	0.005 (3)
N1	0.057 (3)	0.044 (3)	0.044 (3)	0.006 (2)	0.005 (2)	−0.003 (2)
N2	0.053 (3)	0.046 (3)	0.046 (3)	−0.002 (2)	0.007 (3)	−0.003 (2)
C1	0.073 (4)	0.064 (4)	0.051 (4)	0.009 (4)	0.011 (4)	−0.001 (3)
C10	0.073 (4)	0.054 (4)	0.062 (4)	−0.011 (3)	0.006 (4)	−0.006 (3)
C4	0.080 (5)	0.046 (4)	0.073 (5)	0.008 (3)	−0.003 (4)	−0.013 (3)
C9	0.089 (5)	0.082 (5)	0.050 (4)	−0.023 (4)	0.013 (4)	0.004 (4)
C7	0.086 (5)	0.051 (4)	0.070 (5)	−0.013 (4)	0.006 (4)	−0.007 (4)
C2	0.083 (5)	0.090 (6)	0.062 (5)	0.015 (5)	0.022 (5)	−0.010 (4)
C8	0.102 (6)	0.062 (5)	0.071 (5)	−0.023 (4)	0.000 (5)	0.009 (4)
C3	0.094 (6)	0.063 (5)	0.082 (6)	0.027 (4)	0.006 (5)	−0.024 (4)

Geometric parameters (Å, º)

O2—C11	1.252 (7)	C6—C7	1.374 (10)
O2—Co1^{i}	2.126 (4)	N1—C1	1.328 (8)
O4—C12	1.254 (7)	N2—C10	1.327 (9)
O4—Co1^{i}	2.095 (4)	C1—C2	1.379 (10)
C12—O3	1.248 (7)	C1—H1	0.9300
C12—C11	1.541 (6)	C10—C9	1.383 (10)
Co1—O1	2.076 (4)	C10—H10	0.9300
Co1—O4^{ii}	2.095 (4)	C4—C3	1.355 (12)
Co1—O2^{ii}	2.126 (4)	C4—H4	0.9300
Co1—N2	2.139 (5)	C9—C8	1.360 (11)
Co1—O3	2.142 (4)	C9—H9	0.9300
Co1—N1	2.146 (5)	C7—C8	1.379 (11)
C11—O1	1.256 (7)	C7—H7	0.9300
C5—N1	1.336 (8)	C2—C3	1.375 (12)
C5—C4	1.393 (10)	C2—H2	0.9300
C5—C6	1.480 (8)	C8—H8	0.9300
C6—N2	1.354 (8)	C3—H3	0.9300
C11—O2—Co1^{i}	112.6 (4)	C1—N1—C5	118.7 (6)
C12—O4—Co1^{i}	113.4 (4)	C1—N1—Co1	124.9 (5)
O3—C12—O4	126.0 (6)	C5—N1—Co1	116.3 (4)
O3—C12—C11	116.5 (5)	C10—N2—C6	119.1 (6)
O4—C12—C11	117.5 (5)	C10—N2—Co1	125.1 (5)

O1—Co1—O4^{ii}	165.57 (14)	C6—N2—Co1	115.8 (4)
O1—Co1—O2^{ii}	90.30 (17)	N1—C1—C2	122.1 (7)
O4^{ii}—Co1—O2^{ii}	79.14 (16)	N1—C1—H1	119.0
O1—Co1—N2	94.94 (18)	C2—C1—H1	119.0
O4^{ii}—Co1—N2	95.99 (19)	N2—C10—C9	122.5 (7)
O2^{ii}—Co1—N2	96.4 (2)	N2—C10—H10	118.8
O1—Co1—O3	78.61 (16)	C9—C10—H10	118.8
O4^{ii}—Co1—O3	91.91 (17)	C3—C4—C5	118.4 (7)
O2^{ii}—Co1—O3	92.47 (16)	C3—C4—H4	120.8
N2—Co1—O3	169.12 (18)	C5—C4—H4	120.8
O1—Co1—N1	97.18 (19)	C8—C9—C10	119.4 (8)
O4^{ii}—Co1—N1	94.55 (18)	C8—C9—H9	120.3
O2^{ii}—Co1—N1	169.92 (18)	C10—C9—H9	120.3
N2—Co1—N1	76.34 (17)	C6—C7—C8	121.3 (8)
O3—Co1—N1	95.6 (2)	C6—C7—H7	119.3
O2—C11—O1	125.7 (6)	C8—C7—H7	119.3
O2—C11—C12	117.1 (5)	C3—C2—C1	118.8 (8)
O1—C11—C12	117.2 (5)	C3—C2—H2	120.6
C11—O1—Co1	114.6 (4)	C1—C2—H2	120.6
C12—O3—Co1	113.1 (4)	C9—C8—C7	117.8 (7)
N1—C5—C4	122.0 (7)	C9—C8—H8	121.1
N1—C5—C6	115.6 (6)	C7—C8—H8	121.1
C4—C5—C6	122.3 (7)	C4—C3—C2	119.9 (7)
N2—C6—C7	119.8 (7)	C4—C3—H3	120.1
N2—C6—C5	115.8 (6)	C2—C3—H3	120.1
C7—C6—C5	124.3 (7)		

Co1^{i}—O4—C12—O3	−178.1 (5)	O3—Co1—N1—C1	−5.9 (6)
Co1^{i}—O4—C12—C11	3.1 (6)	O1—Co1—N1—C5	97.1 (5)
Co1^{i}—O2—C11—O1	175.8 (5)	O4^{ii}—Co1—N1—C5	−91.3 (5)
Co1^{i}—O2—C11—C12	−4.6 (6)	O2^{ii}—Co1—N1—C5	−40.5 (14)
O3—C12—C11—O2	−177.8 (7)	N2—Co1—N1—C5	3.7 (5)
O4—C12—C11—O2	1.1 (7)	O3—Co1—N1—C5	176.3 (5)
O3—C12—C11—O1	1.8 (7)	C7—C6—N2—C10	2.4 (10)
O4—C12—C11—O1	−179.2 (6)	C5—C6—N2—C10	−178.7 (5)
O2—C11—O1—Co1	178.8 (5)	C7—C6—N2—Co1	−178.0 (6)
C12—C11—O1—Co1	−0.8 (6)	C5—C6—N2—Co1	0.9 (7)
O4^{ii}—Co1—O1—C11	−49.8 (10)	O1—Co1—N2—C10	81.0 (6)
O2^{ii}—Co1—O1—C11	−92.5 (4)	O4^{ii}—Co1—N2—C10	−89.6 (5)
N2—Co1—O1—C11	171.1 (4)	O2^{ii}—Co1—N2—C10	−9.9 (6)
O3—Co1—O1—C11	0.0 (4)	O3—Co1—N2—C10	134.1 (10)
N1—Co1—O1—C11	94.3 (4)	N1—Co1—N2—C10	177.2 (5)
O4—C12—O3—Co1	179.4 (5)	O1—Co1—N2—C6	−98.6 (5)
C11—C12—O3—Co1	−1.8 (6)	O4^{ii}—Co1—N2—C6	90.9 (5)
O1—Co1—O3—C12	1.1 (4)	O2^{ii}—Co1—N2—C6	170.6 (5)
O4^{ii}—Co1—O3—C12	170.1 (4)	O3—Co1—N2—C6	−45.5 (13)
O2^{ii}—Co1—O3—C12	90.9 (4)	N1—Co1—N2—C6	−2.4 (5)
N2—Co1—O3—C12	−53.3 (13)	C5—N1—C1—C2	1.4 (11)

N1—Co1—O3—C12	−95.1 (5)	Co1—N1—C1—C2	−176.3 (6)
N1—C5—C6—N2	2.4 (7)	C6—N2—C10—C9	−1.0 (10)
C4—C5—C6—N2	−179.2 (8)	Co1—N2—C10—C9	179.5 (6)
N1—C5—C6—C7	−178.8 (8)	N1—C5—C4—C3	0.2 (11)
C4—C5—C6—C7	−0.3 (9)	C6—C5—C4—C3	−178.2 (7)
C4—C5—N1—C1	−0.9 (10)	N2—C10—C9—C8	−0.9 (12)
C6—C5—N1—C1	177.6 (6)	N2—C6—C7—C8	−2.1 (12)
C4—C5—N1—Co1	177.1 (5)	C5—C6—C7—C8	179.1 (7)
C6—C5—N1—Co1	−4.5 (7)	N1—C1—C2—C3	−1.3 (12)
O1—Co1—N1—C1	−85.1 (6)	C10—C9—C8—C7	1.2 (13)
O4^{ii}—Co1—N1—C1	86.5 (6)	C6—C7—C8—C9	0.2 (13)
O2^{ii}—Co1—N1—C1	137.3 (11)	C5—C4—C3—C2	0.0 (12)
N2—Co1—N1—C1	−178.4 (6)	C1—C2—C3—C4	0.5 (13)

Symmetry codes: (i) $x+1/2, -y+5/2, z$; (ii) $x-1/2, -y+5/2, z$.