

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

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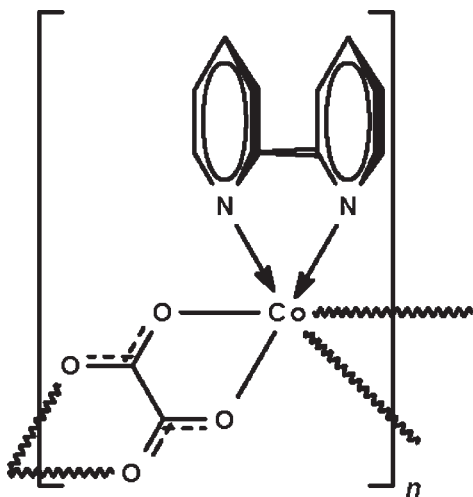
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(C-C) = 0.004$ Å; R factor = 0.026; wR factor = 0.068; data-to-parameter ratio = 15.7.

In the title compound, $[Co(C_2O_4)(C_{10}H_8N_2)]_n$, the oxalate group chelates two adjacent metal atoms, resulting in a zigzag chain running along the a axis. The Co^{II} centre exists in an all cis -octahedral coordination geometry.

Related literature

The Mn(II), Fe(II), Ni(II), Cu(II) and Zn(II) analogs are isostructural; see: Deguenon *et al.* (1990); Fun *et al.* (1999); Lin *et al.* (2006); Luo *et al.* (2001); Yu *et al.* (2006).



Experimental

Crystal data

$[Co(C_2O_4)(C_{10}H_8N_2)]$
 $M_r = 303.13$
 Orthorhombic, $Pna2_1$
 $a = 9.1275$ (8) Å
 $b = 9.2323$ (8) Å
 $c = 14.1929$ (12) Å

$V = 1196.00$ (18) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.45$ mm⁻¹
 $T = 293$ K
 $0.36 \times 0.25 \times 0.18$ mm

Data collection

Bruker APEXII diffractometer
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{min} = 0.624$, $T_{max} = 0.781$

9371 measured reflections
 2698 independent reflections
 2456 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$
 $wR(F^2) = 0.068$
 $S = 1.01$
 2698 reflections
 172 parameters
 1 restraint

H-atom parameters constrained
 $\Delta\rho_{max} = 0.17$ e Å⁻³
 $\Delta\rho_{min} = -0.23$ e Å⁻³
 Absolute structure: Flack (1983),
 1277 Friedel pairs
 Flack parameter: -0.02 (2)

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT (Bruker, 2005); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: X-SEED (Barbour, 2001); software used to prepare material for publication: publCIF (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5061).

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supplementary materials

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catena-Poly[[2,2'-bipyridine- κ^2 N,N']cobalt(II)]- μ -oxalato- κ^4 O¹,O²:O^{1'},O^{2'}]

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Comment

The oxalate group chelates two adjacent metal atoms in $\text{Co}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{C}_2\text{O}_4)$ resulting in a zigzag chain running along the *a*-axis of the orthorhombic unit cell. The cobalt atom exists in an all *cis*-octahedral coordination geometry.

Experimental

An aqueous solution of 2M sodium hydroxide (0.2 ml) was added to a water/DMF (2:7 v/v) solution (9 ml) of cobalt(II) oxalate dihydrate (0.01 g, 0.05 mmol) and 2,2'-bipyridine (0.01 g, 0.05 mmol). Pink blocks separated from the solution after several days in 30% yield. CH&N elemental analysis. Calculated for $\text{C}_{12}\text{H}_8\text{CoN}_2\text{O}_4$: C 47.55, H 2.66, N 9.24%. Found: C 47.27, H 2.94, N 9.40%.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 Å) and were included in the refinement in the riding model approximation, with $U(\text{H})$ set to $1.2U(\text{C})$.

Figures

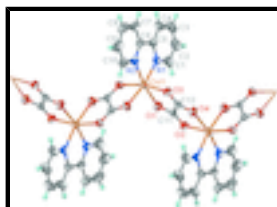


Fig. 1. Anisotropic displacement ellipsoid plot (Barbour, 2001) of a section of the chain structure of $\text{Co}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{C}_2\text{O}_4)$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

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Crystal data

$[\text{Co}(\text{C}_2\text{O}_4)(\text{C}_{10}\text{H}_8\text{N}_2)]$

$M_r = 303.13$

Orthorhombic, *Pna*2₁

Hall symbol: P 2c -2n

$a = 9.1275$ (8) Å

$b = 9.2323$ (8) Å

$c = 14.1929$ (12) Å

$V = 1196.00$ (18) Å³

$F_{000} = 612$

$D_x = 1.683$ Mg m⁻³

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

Cell parameters from 4493 reflections

$\theta = 2.6$ – 26.1°

$\mu = 1.45$ mm⁻¹

$T = 293$ K

Prism, pink

supplementary materials

Z = 4 0.36 × 0.25 × 0.18 mm

Data collection

Bruker APEXII diffractometer	2698 independent reflections
Radiation source: fine-focus sealed tube	2456 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.025$
$T = 293$ K	$\theta_{\text{max}} = 27.5^\circ$
φ and ω scans	$\theta_{\text{min}} = 2.6^\circ$
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	$h = -11 \rightarrow 11$
$T_{\text{min}} = 0.624$, $T_{\text{max}} = 0.781$	$k = -11 \rightarrow 11$
9371 measured reflections	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.026$	$w = 1/[\sigma^2(F_o^2) + (0.0436P)^2]$
$wR(F^2) = 0.068$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{\text{max}} = 0.001$
2698 reflections	$\Delta\rho_{\text{max}} = 0.17 \text{ e } \text{\AA}^{-3}$
172 parameters	$\Delta\rho_{\text{min}} = -0.23 \text{ e } \text{\AA}^{-3}$
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1277 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: -0.02 (2)

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.38104 (3)	0.58866 (2)	0.49966 (4)	0.03408 (9)
N1	0.3016 (2)	0.4155 (2)	0.41608 (15)	0.0413 (5)
N2	0.4481 (2)	0.40387 (19)	0.57666 (14)	0.0390 (4)
O1	0.27899 (18)	0.75569 (19)	0.42055 (11)	0.0445 (4)
O2	0.07533 (18)	0.88996 (17)	0.42286 (12)	0.0409 (4)
O3	0.19137 (17)	0.61940 (16)	0.57821 (11)	0.0389 (3)
O4	-0.00808 (15)	0.75786 (19)	0.58323 (12)	0.0449 (4)
C1	0.2256 (3)	0.4294 (3)	0.3354 (2)	0.0551 (7)
H1	0.1995	0.5218	0.3153	0.066*
C2	0.1847 (3)	0.3113 (4)	0.2810 (2)	0.0674 (8)
H2	0.1334	0.3240	0.2250	0.081*
C3	0.2216 (4)	0.1757 (4)	0.3117 (2)	0.0710 (9)
H3	0.1954	0.0948	0.2765	0.085*
C4	0.2974 (3)	0.1594 (3)	0.3946 (2)	0.0574 (7)

H4	0.3222	0.0675	0.4162	0.069*
C5	0.3367 (3)	0.2817 (3)	0.44589 (16)	0.0385 (5)
C6	0.4169 (3)	0.2747 (3)	0.53643 (18)	0.0390 (5)
C7	0.4574 (4)	0.1460 (3)	0.5795 (2)	0.0583 (7)
H7	0.4359	0.0578	0.5511	0.070*
C8	0.5303 (4)	0.1498 (4)	0.6653 (2)	0.0661 (8)
H8	0.5587	0.0642	0.6947	0.079*
C9	0.5598 (3)	0.2808 (4)	0.70638 (19)	0.0635 (8)
H9	0.6075	0.2857	0.7642	0.076*
C10	0.5172 (3)	0.4054 (3)	0.6601 (2)	0.0531 (7)
H110	0.5373	0.4944	0.6880	0.064*
C11	0.1593 (2)	0.7943 (2)	0.45489 (15)	0.0329 (4)
C12	0.1106 (2)	0.7173 (3)	0.54720 (15)	0.0329 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.03270 (14)	0.03499 (14)	0.03454 (13)	-0.00016 (11)	0.00143 (14)	-0.00307 (16)
N1	0.0463 (11)	0.0436 (11)	0.0339 (10)	-0.0047 (8)	-0.0038 (8)	-0.0021 (8)
N2	0.0408 (11)	0.0406 (11)	0.0356 (10)	0.0037 (8)	-0.0018 (8)	-0.0021 (8)
O1	0.0411 (9)	0.0516 (10)	0.0409 (9)	0.0057 (7)	0.0145 (8)	0.0104 (8)
O2	0.0398 (8)	0.0430 (9)	0.0401 (9)	0.0032 (7)	0.0070 (7)	0.0130 (7)
O3	0.0377 (8)	0.0401 (8)	0.0388 (8)	0.0037 (7)	0.0054 (7)	0.0105 (7)
O4	0.0397 (9)	0.0536 (10)	0.0413 (9)	0.0093 (7)	0.0125 (8)	0.0179 (8)
C1	0.0618 (17)	0.0630 (17)	0.0404 (13)	-0.0075 (13)	-0.0131 (12)	-0.0006 (12)
C2	0.0740 (19)	0.085 (2)	0.0435 (15)	-0.0175 (17)	-0.0170 (14)	-0.0103 (14)
C3	0.082 (2)	0.069 (2)	0.0628 (18)	-0.0255 (17)	-0.0066 (16)	-0.0259 (16)
C4	0.0692 (18)	0.0465 (15)	0.0565 (16)	-0.0145 (13)	-0.0005 (14)	-0.0107 (12)
C5	0.0407 (11)	0.0403 (12)	0.0346 (12)	-0.0044 (11)	0.0034 (10)	-0.0051 (10)
C6	0.0429 (12)	0.0341 (11)	0.0402 (12)	0.0035 (10)	0.0077 (10)	-0.0023 (9)
C7	0.0777 (19)	0.0428 (14)	0.0544 (15)	0.0149 (14)	-0.0004 (15)	-0.0044 (13)
C8	0.086 (2)	0.0576 (17)	0.0546 (16)	0.0271 (16)	0.0024 (16)	0.0105 (15)
C9	0.0727 (18)	0.077 (2)	0.0406 (15)	0.0236 (16)	-0.0064 (13)	0.0052 (14)
C10	0.0622 (17)	0.0555 (16)	0.0416 (13)	0.0124 (12)	-0.0082 (13)	-0.0062 (11)
C11	0.0342 (10)	0.0332 (11)	0.0312 (10)	-0.0055 (10)	0.0024 (9)	0.0017 (9)
C12	0.0318 (11)	0.0349 (11)	0.0321 (11)	-0.0025 (9)	0.0030 (8)	0.0025 (9)

Geometric parameters (\AA , $^\circ$)

Co1—O3	2.0786 (16)	C1—H1	0.9300
Co1—O2 ⁱ	2.0909 (16)	C2—C3	1.367 (5)
Co1—O4 ⁱ	2.1068 (16)	C2—H2	0.9300
Co1—N1	2.119 (2)	C3—C4	1.374 (5)
Co1—N2	2.1165 (19)	C3—H3	0.9300
Co1—O1	2.1228 (17)	C4—C5	1.391 (4)
N1—C1	1.344 (3)	C4—H4	0.9300
N1—C5	1.344 (3)	C5—C6	1.480 (3)
N2—C10	1.342 (3)	C6—C7	1.386 (4)

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N2—C6	1.352 (3)	C7—C8	1.388 (4)
O1—C11	1.248 (3)	C7—H7	0.9300
O2—C11	1.255 (3)	C8—C9	1.369 (5)
O2—Co1 ⁱⁱ	2.0909 (16)	C8—H8	0.9300
O3—C12	1.247 (3)	C9—C10	1.381 (4)
O4—C12	1.255 (2)	C9—H9	0.9300
O4—Co1 ⁱⁱ	2.1068 (16)	C10—H110	0.9300
C1—C2	1.388 (4)	C11—C12	1.555 (2)
O3—Co1—O2 ⁱ	166.68 (6)	C2—C3—C4	119.8 (3)
O3—Co1—O4 ⁱ	90.36 (6)	C2—C3—H3	120.1
O2 ⁱ —Co1—O4 ⁱ	79.78 (6)	C4—C3—H3	120.1
O3—Co1—N1	96.78 (8)	C3—C4—C5	119.3 (3)
O2 ⁱ —Co1—N1	94.00 (7)	C3—C4—H4	120.4
O4 ⁱ —Co1—N1	170.80 (7)	C5—C4—H4	120.4
O3—Co1—N2	94.24 (7)	N1—C5—C4	121.3 (2)
O2 ⁱ —Co1—N2	95.74 (7)	N1—C5—C6	115.6 (2)
O4 ⁱ —Co1—N2	96.46 (8)	C4—C5—C6	123.1 (3)
N1—Co1—N2	77.29 (7)	N2—C6—C7	120.9 (3)
O3—Co1—O1	79.57 (6)	N2—C6—C5	115.6 (2)
O2 ⁱ —Co1—O1	91.60 (7)	C7—C6—C5	123.5 (3)
O4 ⁱ —Co1—O1	91.15 (7)	C8—C7—C6	119.6 (3)
N1—Co1—O1	95.83 (8)	C8—C7—H7	120.2
N2—Co1—O1	170.25 (7)	C6—C7—H7	120.2
C1—N1—C5	118.6 (2)	C9—C8—C7	119.3 (3)
C1—N1—Co1	125.54 (18)	C9—C8—H8	120.3
C5—N1—Co1	115.80 (17)	C7—C8—H8	120.3
C10—N2—C6	118.8 (2)	C8—C9—C10	118.6 (3)
C10—N2—Co1	125.67 (16)	C8—C9—H9	120.7
C6—N2—Co1	115.58 (17)	C10—C9—H9	120.7
C11—O1—Co1	112.63 (14)	N2—C10—C9	122.9 (3)
C11—O2—Co1 ⁱⁱ	113.30 (14)	N2—C10—H110	118.5
C12—O3—Co1	113.72 (14)	C9—C10—H110	118.5
C12—O4—Co1 ⁱⁱ	112.70 (15)	O1—C11—O2	126.4 (2)
N1—C1—C2	122.5 (3)	O1—C11—C12	116.67 (18)
N1—C1—H1	118.8	O2—C11—C12	116.88 (17)
C2—C1—H1	118.8	O3—C12—O4	125.7 (2)
C3—C2—C1	118.5 (3)	O3—C12—C11	117.35 (17)
C3—C2—H2	120.8	O4—C12—C11	116.98 (18)
C1—C2—H2	120.8		
O3—Co1—N1—C1	86.2 (2)	C1—N1—C5—C6	-178.5 (2)
O2 ⁱ —Co1—N1—C1	-86.0 (2)	Co1—N1—C5—C6	4.1 (3)
N2—Co1—N1—C1	179.0 (2)	C3—C4—C5—N1	0.2 (4)
O1—Co1—N1—C1	6.0 (2)	C3—C4—C5—C6	179.3 (3)
O3—Co1—N1—C5	-96.68 (18)	C10—N2—C6—C7	-1.1 (4)
O2 ⁱ —Co1—N1—C5	91.16 (18)	Co1—N2—C6—C7	179.0 (2)

N2—Co1—N1—C5	-3.84 (18)	C10—N2—C6—C5	178.2 (2)
O1—Co1—N1—C5	-176.83 (18)	Co1—N2—C6—C5	-1.7 (3)
O3—Co1—N2—C10	-81.0 (2)	N1—C5—C6—N2	-1.6 (3)
O2 ⁱ —Co1—N2—C10	90.2 (2)	C4—C5—C6—N2	179.2 (3)
O4 ⁱ —Co1—N2—C10	9.8 (2)	N1—C5—C6—C7	177.7 (3)
N1—Co1—N2—C10	-177.0 (2)	C4—C5—C6—C7	-1.5 (4)
O3—Co1—N2—C6	98.92 (19)	N2—C6—C7—C8	0.4 (5)
O2 ⁱ —Co1—N2—C6	-89.91 (18)	C5—C6—C7—C8	-178.9 (2)
O4 ⁱ —Co1—N2—C6	-170.23 (18)	C6—C7—C8—C9	0.5 (5)
N1—Co1—N2—C6	2.91 (19)	C7—C8—C9—C10	-0.7 (5)
O3—Co1—O1—C11	0.09 (16)	C6—N2—C10—C9	0.9 (4)
O2 ⁱ —Co1—O1—C11	-169.87 (16)	Co1—N2—C10—C9	-179.2 (2)
O4 ⁱ —Co1—O1—C11	-90.06 (16)	C8—C9—C10—N2	0.0 (4)
N1—Co1—O1—C11	95.94 (17)	Co1—O1—C11—O2	-179.71 (19)
O2 ⁱ —Co1—O3—C12	47.6 (4)	Co1—O1—C11—C12	1.1 (2)
O4 ⁱ —Co1—O3—C12	89.55 (17)	Co1 ⁱⁱ —O2—C11—O1	177.06 (19)
N1—Co1—O3—C12	-96.27 (17)	Co1 ⁱⁱ —O2—C11—C12	-3.8 (2)
N2—Co1—O3—C12	-173.95 (17)	Co1—O3—C12—O4	-178.58 (19)
O1—Co1—O3—C12	-1.55 (16)	Co1—O3—C12—C11	2.6 (2)
C5—N1—C1—C2	-1.3 (4)	Co1 ⁱⁱ —O4—C12—O3	-174.00 (19)
Co1—N1—C1—C2	175.8 (2)	Co1 ⁱⁱ —O4—C12—C11	4.9 (2)
N1—C1—C2—C3	0.9 (5)	O1—C11—C12—O3	-2.6 (3)
C1—C2—C3—C4	0.0 (5)	O2—C11—C12—O3	178.2 (2)
C2—C3—C4—C5	-0.5 (5)	O1—C11—C12—O4	178.4 (2)
C1—N1—C5—C4	0.7 (4)	O2—C11—C12—O4	-0.8 (3)
Co1—N1—C5—C4	-176.7 (2)		

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

Fig. 1

