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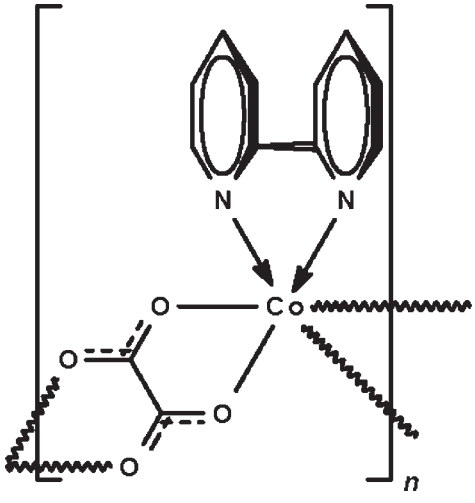
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.026; wR factor = 0.068; data-to-parameter ratio = 15.7.

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) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.45 mm^{-1}
T = 293 K
0.36 × 0.25 × 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).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2005). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Deguenon, D., Bernardinelli, G., Tucahgues, J. P. & Castan, P. (1990). *Inorg. Chem.* **29**, 3031–3037.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Fun, H.-K., Shanmuga Sundara Raj, S., Fang, X., Zheng, L.-M. & Xin, X.-Q. (1999). *Acta Cryst.* C**55**, 903–905.
Lin, X.-R., Ye, B.-Z., Liu, J.-S., Wei, C.-X. & Chen, J.-X. (2006). *Acta Cryst.* E**62**, m2130–m2132.
Luo, J.-H., Hong, M.-C., Liang, Y.-C. & Cao, R. (2001). *Acta Cryst.* E**57**, m361–m362.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2009). *publCIF*. In preparation.
Yu, J.-H., Bi, M.-H., Lu, Z.-L., Zhang, X., Qu, X.-J., Lu, J. & Xu, J.-Q. (2006). *J. Mol. Struct.* **800**, 69–73.

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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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S1. Comment

The oxalate group chelates two adjacent metal atoms in $Co(C_{10}H_8N_2)(C_2O_4)$ 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.

S2. Experimental

An aqueous solution of 2*M* sodium hydroxide (0.2 ml) was added to a water/DMF (2:7 *v*/*v*) solution (9 ml) of cobalt(II) oxalate dihdyrate (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 $C_{12}H_8CoN_2O_4$: C 47.55, H 2.66, N 9.24%. Found: C 47.27, H 2.94, N 9.40%.

S3. 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*(H) set to 1.2*U*(C).

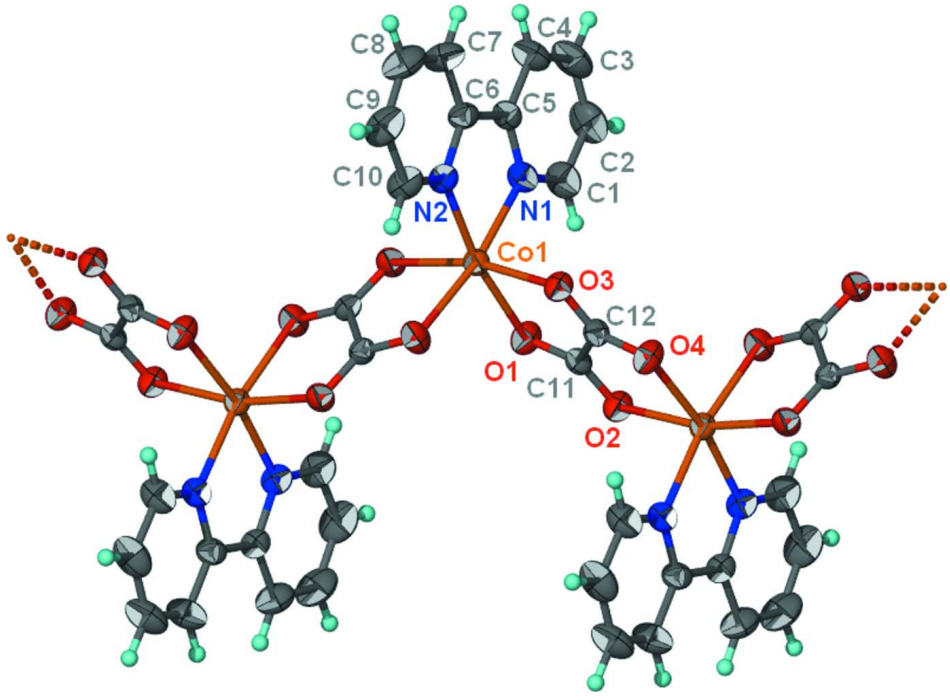

Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of a section of the chain structure of $Co(C_{10}H_8N_2)(C_2O_4)$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

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Crystal data

$[Co(C_2O_4)(C_{10}H_8N_2)]$
$M_r = 303.13$
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 9.1275$ (8) Å
$b = 9.2323$ (8) Å
$c = 14.1929$ (12) Å
$V = 1196.00$ (18) Å^3
$Z = 4$
$F(000) = 612$
$D_x = 1.683$ 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
0.36 × 0.25 × 0.18 mm

Data collection

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

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.068$
$S = 1.01$
2698 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
$w = 1/[\sigma^2(F_o^2) + (0.0436P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}
Absolute structure: Flack (1983), 1277 Friedel pairs
Absolute structure parameter: −0.02 (2)

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

	x	*y*	*z*	U_{iso}*/U_{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 (Å²)

	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 (Å, º)

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)
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) $x-1/2, -y+3/2, z$.