

catena-Poly[[bis(acetato- κ^2O,O')-cobalt(II)]- μ -4,4'-bis(benzimidazol-1-yl)-biphenyl- $\kappa^2N^3:N^{3'}$]

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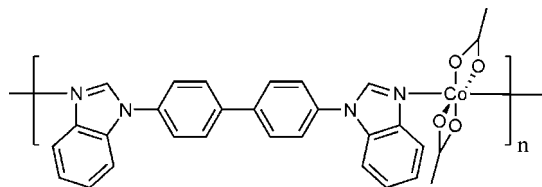
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(C-C) = 0.003$ Å; R factor = 0.035; wR factor = 0.083; data-to-parameter ratio = 12.1.

In the title one-dimensional coordination polymer, $[Co(C_2H_3O_2)_2(C_{26}H_{18}N_4)]_n$, the Co^{II} atom (site symmetry 2) is coordinated by two O,O' -bidentate acetate ions and two 4,4'-bis(benzimidazol-1-yl)biphenyl ligands in a distorted $cis-CoN_2O_4$ octahedral geometry. The bridging ligand, which is completed by crystallographic twofold symmetry, links the Co^{II} atoms into $[10\bar{1}]$ chains. Within the ligand, the dihedral angle between the benzene and benzimidazole rings is $48.31(8)^\circ$.

Related literature

For background to benzimidazole-derived ligands in coordination polymers, see: Jin *et al.* (2006); Li *et al.* (2010); Su *et al.* (2003).



Experimental

Crystal data

$[Co(C_2H_3O_2)_2(C_{26}H_{18}N_4)]$
 $M_r = 563.46$
 Orthorhombic, $Pbcn$
 $a = 13.078(3)$ Å
 $b = 16.348(3)$ Å
 $c = 11.354(2)$ Å
 $V = 2427.5(8)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.75$ mm⁻¹
 $T = 293$ K
 $0.25 \times 0.22 \times 0.18$ mm

Data collection

Rigaku CCD area-detector diffractometer
 Absorption correction: multi-scan (*CrystalClear*; Rigaku/MS, 2005)
 $T_{min} = 0.828$, $T_{max} = 0.873$
 21778 measured reflections
 2150 independent reflections
 2101 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.038$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.083$
 $S = 1.10$
 2150 reflections
 178 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 0.27$ e Å⁻³
 $\Delta\rho_{min} = -0.41$ e Å⁻³

Table 1

Selected bond lengths (Å).

Co1—O1	2.0386 (16)	Co1—N1	2.0709 (16)
Co1—O2	2.4163 (18)		

Data collection: *CrystalClear* (Rigaku/MS, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5708).

References

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supplementary materials

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P.-Y. Huang and J.-G. Wang

Comment

Benzoimidazole has been well used in crystal engineering, and a large number of benzoimidazole-containing flexible ligands have been extensively studied (Su *et al.*,2003; Jin *et al.*,2006). However, to our knowledge, the research on benzoimidazole ligands bearing rigid spacers is still less developed (Li *et al.*,2010).

Single-crystal X-ray diffraction analysis reveals that the title compound (**I**) crystallizes in the orthorhombic space group *Pbcn*. The geometry of the Co^{II} ion is surrounded by two benzoimidazole rings of distinct **L** ligands and two chelated acetate anions, which illustrates a slightly distorted octahedral coordination environment (Fig. 1). Notably, as shown in Fig. 2, the six-coordinated Co^{II} center is bridged by the linear ligand **L** to form an infinite one-dimensional architecture.

Experimental

A mixture of CH₃OH and CHCl₃ (1:1, 8 ml), as a buffer layer, was carefully layered over a solution of 4,4'-bis(benzoimidazol-1-yl)terphenyl (**L**, 0.06 mmol) in CHCl₃ (6 ml). Then a solution of Co(CH₃COO)₂ (0.02 mmol) in CH₃OH (6 ml) was layered over the buffer layer, and the resultant reaction was left to stand at room temperature. After *ca* three weeks, purple blocks of (**I**) appeared at the boundary. Yield: ~25% (based on **L**).

Refinement

C-bound H atoms were positioned geometrically and refined in the riding-model approximation, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$.

Figures

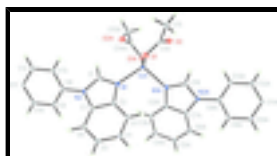


Fig. 1. The molecular structure of (**I**). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius.

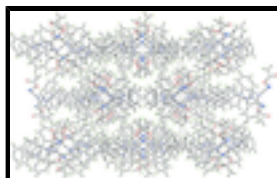


Fig. 2. The crystal packing for (**I**).

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Crystal data

$[\text{Co}(\text{C}_2\text{H}_3\text{O}_2)_2(\text{C}_{26}\text{H}_{18}\text{N}_4)]$	$D_x = 1.542 \text{ Mg m}^{-3}$
$M_r = 563.46$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Orthorhombic, $Pbcn$	Cell parameters from 6002 reflections
$a = 13.078 (3) \text{ \AA}$	$\theta = 2.0\text{--}27.9^\circ$
$b = 16.348 (3) \text{ \AA}$	$\mu = 0.75 \text{ mm}^{-1}$
$c = 11.354 (2) \text{ \AA}$	$T = 293 \text{ K}$
$V = 2427.5 (8) \text{ \AA}^3$	Block, purple
$Z = 4$	$0.25 \times 0.22 \times 0.18 \text{ mm}$
$F(000) = 1164$	

Data collection

Rigaku CCD area-detector diffractometer	2150 independent reflections
Radiation source: fine-focus sealed tube graphite	2101 reflections with $I > 2\sigma(I)$
Detector resolution: 9 pixels mm^{-1}	$R_{\text{int}} = 0.038$
ω scans	$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.7^\circ$
Absorption correction: multi-scan (<i>CrystalClear</i> ; Rigaku/MS, 2005)	$h = -15 \rightarrow 15$
$T_{\text{min}} = 0.828$, $T_{\text{max}} = 0.873$	$k = -19 \rightarrow 19$
21778 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.035$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.083$	H-atom parameters constrained
$S = 1.10$	$w = 1/[\sigma^2(F_o^2) + (0.0367P)^2 + 2.7447P]$
2150 reflections	where $P = (F_o^2 + 2F_c^2)/3$
178 parameters	$(\Delta/\sigma)_{\text{max}} < 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.27 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.41 \text{ e \AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.0000	0.40968 (2)	0.2500	0.01345 (14)
O1	0.08394 (11)	0.37040 (10)	0.39033 (14)	0.0268 (4)
C11	0.45996 (14)	0.51680 (12)	-0.20359 (17)	0.0138 (4)
C12	0.44299 (15)	0.44856 (12)	-0.13277 (18)	0.0160 (4)
H12	0.4800	0.4009	-0.1461	0.019*
C7	0.23045 (15)	0.58691 (12)	0.15147 (17)	0.0134 (4)
C3	0.11760 (15)	0.61095 (13)	0.31741 (17)	0.0163 (4)
H3	0.0633	0.5956	0.3655	0.020*
N2	0.24267 (12)	0.52419 (10)	0.06971 (14)	0.0140 (4)
N1	0.11225 (12)	0.48650 (10)	0.18429 (14)	0.0148 (4)
C10	0.40024 (15)	0.58655 (13)	-0.18495 (18)	0.0171 (4)
H10	0.4096	0.6322	-0.2327	0.021*
C13	0.37154 (15)	0.45080 (12)	-0.04256 (18)	0.0162 (4)
H13	0.3618	0.4054	0.0055	0.019*
C8	0.31481 (14)	0.52118 (12)	-0.02460 (17)	0.0144 (4)
C9	0.32729 (15)	0.58878 (12)	-0.09655 (18)	0.0164 (4)
H9	0.2872	0.6351	-0.0857	0.020*
C14	0.02557 (15)	0.31459 (12)	0.42490 (18)	0.0163 (4)
O2	-0.06065 (12)	0.30382 (10)	0.38106 (15)	0.0292 (4)
C4	0.17056 (15)	0.68295 (13)	0.33635 (18)	0.0184 (4)
H4	0.1517	0.7165	0.3989	0.022*
C1	0.17101 (15)	0.46685 (12)	0.09472 (17)	0.0153 (4)
H1	0.1641	0.4184	0.0526	0.018*
C15	0.06315 (17)	0.25921 (14)	0.5229 (2)	0.0249 (5)
H15A	0.0636	0.2889	0.5958	0.037*
H15B	0.1312	0.2408	0.5052	0.037*
H15C	0.0185	0.2128	0.5297	0.037*
C2	0.14891 (15)	0.56223 (12)	0.22333 (17)	0.0140 (4)
C6	0.28339 (15)	0.65947 (12)	0.16999 (17)	0.0162 (4)
H6	0.3372	0.6753	0.1216	0.019*
C5	0.25205 (16)	0.70673 (13)	0.26368 (18)	0.0176 (4)
H5	0.2858	0.7557	0.2792	0.021*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0112 (2)	0.0150 (2)	0.0141 (2)	0.000	0.00353 (14)	0.000

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O1	0.0208 (8)	0.0286 (9)	0.0311 (9)	-0.0010 (7)	0.0001 (7)	0.0116 (7)
C11	0.0112 (9)	0.0182 (11)	0.0121 (9)	-0.0018 (8)	0.0014 (8)	-0.0006 (8)
C12	0.0148 (10)	0.0151 (10)	0.0182 (10)	0.0020 (8)	0.0026 (8)	-0.0013 (8)
C7	0.0132 (10)	0.0144 (10)	0.0126 (9)	0.0016 (7)	0.0007 (8)	0.0005 (8)
C3	0.0146 (10)	0.0214 (11)	0.0131 (10)	0.0008 (8)	0.0029 (8)	0.0006 (8)
N2	0.0134 (8)	0.0153 (8)	0.0133 (8)	-0.0009 (6)	0.0049 (7)	-0.0002 (7)
N1	0.0145 (8)	0.0154 (9)	0.0146 (8)	-0.0018 (7)	0.0037 (7)	-0.0016 (7)
C10	0.0173 (10)	0.0173 (11)	0.0167 (10)	0.0001 (8)	0.0041 (8)	0.0032 (8)
C13	0.0176 (10)	0.0144 (10)	0.0166 (10)	-0.0023 (8)	0.0035 (8)	0.0012 (8)
C8	0.0109 (9)	0.0189 (10)	0.0135 (10)	-0.0017 (8)	0.0042 (8)	-0.0012 (8)
C9	0.0141 (10)	0.0166 (10)	0.0184 (10)	0.0031 (8)	0.0036 (8)	0.0001 (8)
C14	0.0138 (10)	0.0187 (10)	0.0165 (10)	0.0023 (8)	0.0040 (8)	-0.0055 (8)
O2	0.0279 (9)	0.0226 (8)	0.0372 (9)	-0.0004 (7)	-0.0079 (8)	-0.0027 (7)
C4	0.0200 (11)	0.0197 (11)	0.0154 (10)	0.0025 (8)	0.0005 (8)	-0.0043 (8)
C1	0.0139 (10)	0.0159 (10)	0.0162 (10)	-0.0007 (8)	0.0038 (8)	-0.0009 (8)
C15	0.0237 (12)	0.0244 (12)	0.0265 (12)	0.0012 (9)	0.0015 (9)	0.0031 (10)
C2	0.0126 (9)	0.0151 (10)	0.0144 (10)	0.0010 (8)	0.0004 (8)	0.0007 (8)
C6	0.0129 (9)	0.0176 (10)	0.0180 (10)	-0.0015 (8)	0.0020 (8)	0.0019 (8)
C5	0.0162 (10)	0.0147 (10)	0.0220 (11)	-0.0014 (8)	-0.0022 (8)	-0.0016 (8)

Geometric parameters (Å, °)

Co1—O1 ⁱ	2.0386 (16)	N1—C1	1.315 (3)
Co1—O1	2.0386 (16)	N1—C2	1.400 (3)
Co1—O2	2.4163 (18)	C10—C9	1.385 (3)
Co1—O2 ⁱ	2.4163 (18)	C10—H10	0.9300
Co1—N1	2.0709 (16)	C13—C8	1.384 (3)
Co1—N1 ⁱ	2.0709 (16)	C13—H13	0.9300
O1—C14	1.253 (3)	C8—C9	1.384 (3)
C11—C12	1.393 (3)	C9—H9	0.9300
C11—C10	1.398 (3)	C14—O2	1.245 (3)
C11—C11 ⁱⁱ	1.486 (4)	C14—C15	1.516 (3)
C12—C13	1.387 (3)	C4—C5	1.403 (3)
C12—H12	0.9300	C4—H4	0.9300
C7—C6	1.390 (3)	C1—H1	0.9300
C7—N2	1.392 (2)	C15—H15A	0.9600
C7—C2	1.402 (3)	C15—H15B	0.9600
C3—C4	1.383 (3)	C15—H15C	0.9600
C3—C2	1.394 (3)	C6—C5	1.377 (3)
C3—H3	0.9300	C6—H6	0.9300
N2—C1	1.356 (3)	C5—H5	0.9300
N2—C8	1.428 (2)		
O1 ⁱ —Co1—O1	143.29 (10)	C9—C8—C13	120.90 (18)
O1 ⁱ —Co1—N1	106.93 (7)	C9—C8—N2	119.55 (17)
O1—Co1—N1	95.21 (6)	C13—C8—N2	119.55 (17)
O1 ⁱ —Co1—N1 ⁱ	95.21 (6)	C8—C9—C10	119.21 (18)
O1—Co1—N1 ⁱ	106.93 (7)	C8—C9—H9	120.4

N1—Co1—N1 ⁱ	105.34 (9)	C10—C9—H9	120.4
C14—O1—Co1	98.41 (13)	O2—C14—O1	122.0 (2)
C12—C11—C10	118.47 (18)	O2—C14—C15	120.16 (19)
C12—C11—C11 ⁱⁱ	121.45 (13)	O1—C14—C15	117.86 (18)
C10—C11—C11 ⁱⁱ	120.07 (13)	C3—C4—C5	121.67 (19)
C13—C12—C11	120.84 (18)	C3—C4—H4	119.2
C13—C12—H12	119.6	C5—C4—H4	119.2
C11—C12—H12	119.6	N1—C1—N2	113.41 (18)
C6—C7—N2	132.25 (18)	N1—C1—H1	123.3
C6—C7—C2	122.45 (18)	N2—C1—H1	123.3
N2—C7—C2	105.27 (17)	C14—C15—H15A	109.5
C4—C3—C2	117.29 (18)	C14—C15—H15B	109.5
C4—C3—H3	121.4	H15A—C15—H15B	109.5
C2—C3—H3	121.4	C14—C15—H15C	109.5
C1—N2—C7	106.87 (16)	H15A—C15—H15C	109.5
C1—N2—C8	126.16 (17)	H15B—C15—H15C	109.5
C7—N2—C8	126.95 (16)	C3—C2—N1	130.35 (18)
C1—N1—C2	105.12 (16)	C3—C2—C7	120.32 (19)
C1—N1—Co1	123.02 (14)	N1—C2—C7	109.32 (17)
C2—N1—Co1	131.69 (13)	C5—C6—C7	116.59 (18)
C9—C10—C11	121.05 (19)	C5—C6—H6	121.7
C9—C10—H10	119.5	C7—C6—H6	121.7
C11—C10—H10	119.5	C6—C5—C4	121.67 (19)
C8—C13—C12	119.46 (18)	C6—C5—H5	119.2
C8—C13—H13	120.3	C4—C5—H5	119.2
C12—C13—H13	120.3		
O1 ⁱ —Co1—O1—C14	-43.39 (12)	C13—C8—C9—C10	-2.3 (3)
N1—Co1—O1—C14	-171.08 (13)	N2—C8—C9—C10	177.49 (18)
N1 ⁱ —Co1—O1—C14	81.14 (14)	C11—C10—C9—C8	1.1 (3)
C10—C11—C12—C13	-2.7 (3)	Co1—O1—C14—O2	-6.9 (2)
C11 ⁱⁱ —C11—C12—C13	176.7 (2)	Co1—O1—C14—C15	172.84 (15)
C6—C7—N2—C1	178.2 (2)	C2—C3—C4—C5	0.5 (3)
C2—C7—N2—C1	0.0 (2)	C2—N1—C1—N2	-1.1 (2)
C6—C7—N2—C8	-3.3 (3)	Co1—N1—C1—N2	-176.94 (13)
C2—C7—N2—C8	178.53 (18)	C7—N2—C1—N1	0.7 (2)
O1 ⁱ —Co1—N1—C1	-49.07 (17)	C8—N2—C1—N1	-177.81 (17)
O1—Co1—N1—C1	101.29 (16)	C4—C3—C2—N1	178.6 (2)
N1 ⁱ —Co1—N1—C1	-149.55 (18)	C4—C3—C2—C7	-0.5 (3)
O1 ⁱ —Co1—N1—C2	136.34 (17)	C1—N1—C2—C3	-178.1 (2)
O1—Co1—N1—C2	-73.29 (18)	Co1—N1—C2—C3	-2.8 (3)
N1 ⁱ —Co1—N1—C2	35.86 (15)	C1—N1—C2—C7	1.1 (2)
C12—C11—C10—C9	1.4 (3)	Co1—N1—C2—C7	176.39 (13)
C11 ⁱⁱ —C11—C10—C9	-178.0 (2)	C6—C7—C2—C3	0.2 (3)
C11—C12—C13—C8	1.5 (3)	N2—C7—C2—C3	178.57 (17)
C12—C13—C8—C9	1.0 (3)	C6—C7—C2—N1	-179.06 (18)
C12—C13—C8—N2	-178.74 (17)	N2—C7—C2—N1	-0.7 (2)

supplementary materials

C1—N2—C8—C9	131.6 (2)	N2—C7—C6—C5	-177.7 (2)
C7—N2—C8—C9	-46.6 (3)	C2—C7—C6—C5	0.2 (3)
C1—N2—C8—C13	-48.6 (3)	C7—C6—C5—C4	-0.3 (3)
C7—N2—C8—C13	133.1 (2)	C3—C4—C5—C6	-0.1 (3)

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

Fig. 1

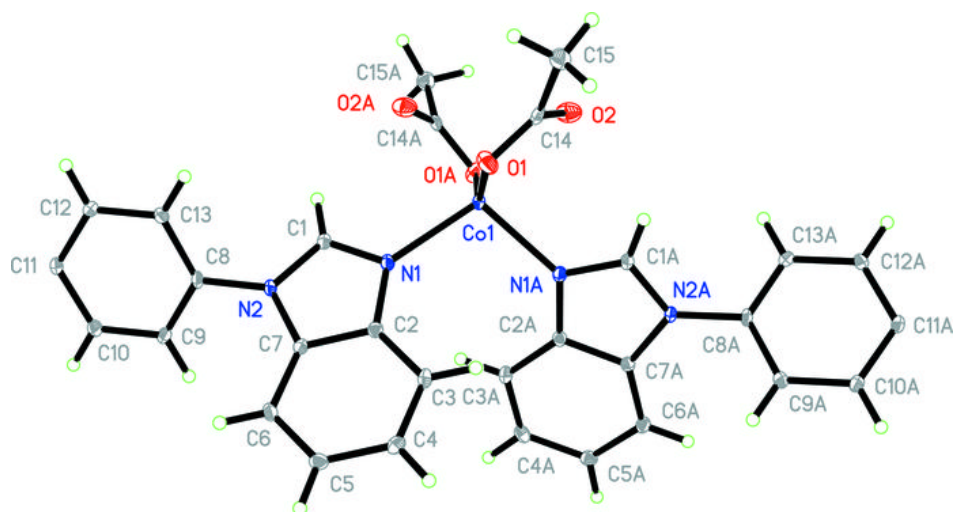


Fig. 2

