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Bis(isocyanato-κN)bis(1,10-phenanthroline-$\kappa^2 N,N'$)cobalt(II)

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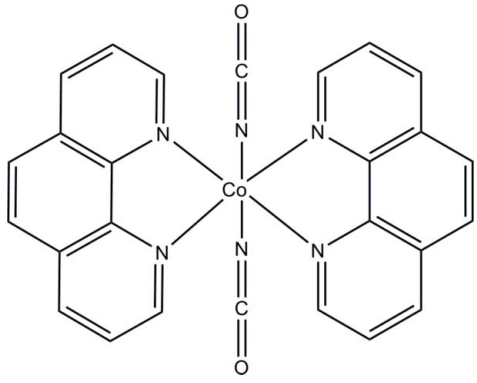
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.044; wR factor = 0.144; data-to-parameter ratio = 11.9.

In the title complex, $[Co(NCO)_2(C_{12}H_8N_2)_2]$, the Co^{II} atom, lying on a twofold rotation axis, is coordinated in a distorted octahedral environment by four N atoms from two chelating phenanthroline ligands and two N atoms from two isocyanate ligands in *cis* positions.

Related literature

For related structures, see: Cheng & Hu (2003); He *et al.* (2004); Yin (2007).



Experimental

Crystal data

$[Co(CNO)_2(C_{12}H_8N_2)_2]$
M_r = 503.38
Orthorhombic, *Pbcn*
a = 13.2317 (8) Å
b = 9.7095 (6) Å
c = 16.7265 (10) Å
V = 2148.9 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.84 mm^{-1}
T = 293 K
0.27 × 0.25 × 0.18 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.805, T_{max} = 0.864
9949 measured reflections
1890 independent reflections
1553 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.144
S = 1.06
1890 reflections
159 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—N1	2.168 (2)	Co1—N3	2.058 (3)
Co1—N2	2.223 (3)		

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT-Plus* (Bruker, 2007); data reduction: *SAINT-Plus* (Bruker, 2007); 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: HY2302).

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supplementary materials

Acta Cryst. (2010). E**66**, m614 [**doi:10.1107/S1600536810015758**]

Bis(isocyanato-κN)bis(1,10-phenanthroline-$\kappa^2 N,N'$)cobalt(II)

D.-P. Zhang, N.-C. Tian and X.-M. Zhang

Comment

As has been known for a very long time, 1,10-phenanthroline (phen) is a good bidentate chelating ligand, and has been widely introduced into the transition metal complexes. Here, we present a new six-coordinated cobalt(II) complex based on phen.

The molecular structure of the title compound is shown in Fig. 1. The coordination geometry of the Co^{II} ion is distorted octahedral, in which four positions are occupied by four N atoms of two chelating phen ligands and the other two occupied by two N atoms of two isocyanate ligands at a *cis* position. The Co—N_{phen} and Co—$N_{isocyanate}$ bond lengths are 2.168 (2), 2.223 (3) and 2.058 (3) Å (Table 1), respectively, which are all comparable to those found in other bis(phen)cobalt(II) complexes (Cheng & Hu, 2003; He *et al.*, 2004; Yin, 2007).

Experimental

To a solution of 1,10-phenanthroline monohydrate (39.6 mg, 0.2 mmol) dissolved in methanol (15 ml) was added $Co(ClO_4)_2.6H_2O$ (36.6 mg, 0.1 mmol). The mixture was stirred for 5 min before NaNCO (13 mg, 0.2 mmol) was added. After the stirring process was continued for an additional 5 min, the mixture was filtered, and the filtrate was allowed to slow evaporate to afford orange-yellow crystals suitable for X-ray diffraction with a yield about 55%.

Refinement

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

Figures

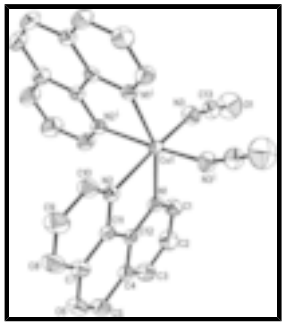


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. H atoms are omitted for clarity. [Symmetry code: (i) 1-x, y, 3/2-z.]

Bis(isocyanato-κ*N*)bis(1,10-phenanthroline- κ^2N,N')cobalt(II)

Crystal data

$[Co(CNO)_2(C_{12}H_8N_2)_2]$	$F(000) = 1028$
$M_r = 503.38$	$D_x = 1.556$ Mg m^{-3}
Orthorhombic, *Pbcn*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -P 2n 2ab	Cell parameters from 1231 reflections
$a = 13.2317$ (8) Å	θ = 2.6–27.0°
$b = 9.7095$ (6) Å	μ = 0.84 mm^{-1}
$c = 16.7265$ (10) Å	$T = 293$ K
$V = 2148.9$ (2) Å^3	Block, orange-yellow
$Z = 4$	0.27 × 0.25 × 0.18 mm

Data collection

Bruker APEXII CCD diffractometer	1890 independent reflections
Radiation source: fine-focus sealed tube	1553 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.023$
φ and ω scans	$\theta_{max} = 25.0°$, $\theta_{min} = 2.4°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -15\rightarrow15$
$T_{min} = 0.805$, $T_{max} = 0.864$	$k = -7\rightarrow11$
9949 measured reflections	$l = -19\rightarrow19$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.044$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.144$	H-atom parameters constrained
$S = 1.06$	$w = 1/[\sigma^2(F_o^2) + (0.0851P)^2 + 1.8714P]$ where $P = (F_o^2 + 2F_c^2)/3$
1890 reflections	$(\Delta/\sigma)_{max} = 0.001$
159 parameters	$\Delta\rho_{max} = 0.70$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.62$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.5000	0.18820 (5)	0.7500	0.0357 (2)
O1	0.3547 (3)	0.4750 (4)	0.9117 (2)	0.1113 (12)
N1	0.34514 (17)	0.1463 (3)	0.71529 (15)	0.0407 (6)

N2	0.51307 (17)	0.0223 (3)	0.65894 (15)	0.0402 (6)
N3	0.4590 (2)	0.3270 (3)	0.83709 (18)	0.0551 (7)
C1	0.2633 (3)	0.2026 (4)	0.7466 (2)	0.0519 (9)
H1	0.2713	0.2725	0.7841	0.062*
C2	0.1656 (3)	0.1624 (4)	0.7262 (3)	0.0636 (10)
H2	0.1099	0.2033	0.7503	0.076*
C3	0.1531 (3)	0.0611 (4)	0.6696 (3)	0.0694 (11)
H3	0.0886	0.0323	0.6553	0.083*
C4	0.2379 (2)	0.0016 (3)	0.6335 (2)	0.0507 (8)
C5	0.2324 (3)	−0.1020 (4)	0.5729 (3)	0.0721 (11)
H5	0.1695	−0.1280	0.5532	0.086*
C6	0.3168 (3)	−0.1634 (4)	0.5432 (2)	0.0705 (11)
H6	0.3108	−0.2326	0.5050	0.085*
C7	0.4141 (3)	−0.1225 (4)	0.5701 (2)	0.0581 (9)
C8	0.5032 (3)	−0.1852 (5)	0.5447 (3)	0.0720 (14)
H8	0.5003	−0.2574	0.5082	0.086*
C9	0.5947 (3)	−0.1417 (5)	0.5727 (2)	0.0759 (12)
H9	0.6545	−0.1807	0.5542	0.091*
C10	0.5961 (3)	−0.0358 (4)	0.6307 (2)	0.0548 (8)
H10	0.6583	−0.0057	0.6499	0.066*
C11	0.4227 (2)	−0.0189 (3)	0.62939 (17)	0.0402 (7)
C12	0.3333 (2)	0.0450 (3)	0.65996 (17)	0.0410 (7)
C13	0.4114 (3)	0.4017 (4)	0.8731 (2)	0.0548 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0293 (4)	0.0381 (4)	0.0396 (4)	0.000	−0.0021 (2)	0.000
O1	0.112 (3)	0.117 (3)	0.105 (3)	0.031 (2)	0.026 (2)	−0.026 (2)
N1	0.0337 (13)	0.0439 (13)	0.0446 (14)	−0.0007 (11)	−0.0062 (11)	0.0051 (11)
N2	0.0395 (13)	0.0402 (14)	0.0409 (13)	0.0017 (10)	−0.0029 (10)	−0.0013 (11)
N3	0.0524 (17)	0.0535 (16)	0.0593 (17)	0.0016 (13)	0.0047 (15)	−0.0093 (14)
C1	0.0381 (19)	0.055 (2)	0.062 (2)	0.0014 (15)	−0.0010 (13)	−0.0053 (15)
C2	0.0308 (17)	0.068 (2)	0.092 (3)	−0.0021 (16)	0.0034 (18)	0.002 (2)
C3	0.0423 (19)	0.071 (2)	0.095 (3)	−0.0157 (18)	−0.0190 (19)	0.004 (2)
C4	0.0464 (18)	0.0461 (17)	0.0598 (19)	−0.0053 (14)	−0.0155 (15)	0.0057 (15)
C5	0.065 (2)	0.071 (2)	0.080 (3)	−0.020 (2)	−0.032 (2)	−0.004 (2)
C6	0.080 (3)	0.064 (2)	0.067 (2)	−0.015 (2)	−0.021 (2)	−0.0126 (19)
C7	0.070 (2)	0.058 (2)	0.0467 (18)	−0.0031 (18)	−0.0113 (17)	−0.0070 (16)
C8	0.073 (3)	0.081 (3)	0.062 (3)	0.0094 (19)	−0.0093 (18)	−0.032 (2)
C9	0.073 (3)	0.095 (3)	0.060 (2)	0.021 (2)	0.000 (2)	−0.030 (2)
C10	0.0512 (19)	0.060 (2)	0.0529 (19)	0.0070 (16)	−0.0040 (15)	−0.0139 (16)
C11	0.0435 (16)	0.0374 (15)	0.0398 (15)	−0.0038 (12)	−0.0097 (13)	0.0058 (12)
C12	0.0440 (16)	0.0365 (14)	0.0426 (15)	−0.0042 (12)	−0.0106 (13)	0.0112 (12)
C13	0.055 (2)	0.0567 (19)	0.0525 (19)	0.0017 (17)	0.0092 (16)	−0.0045 (16)

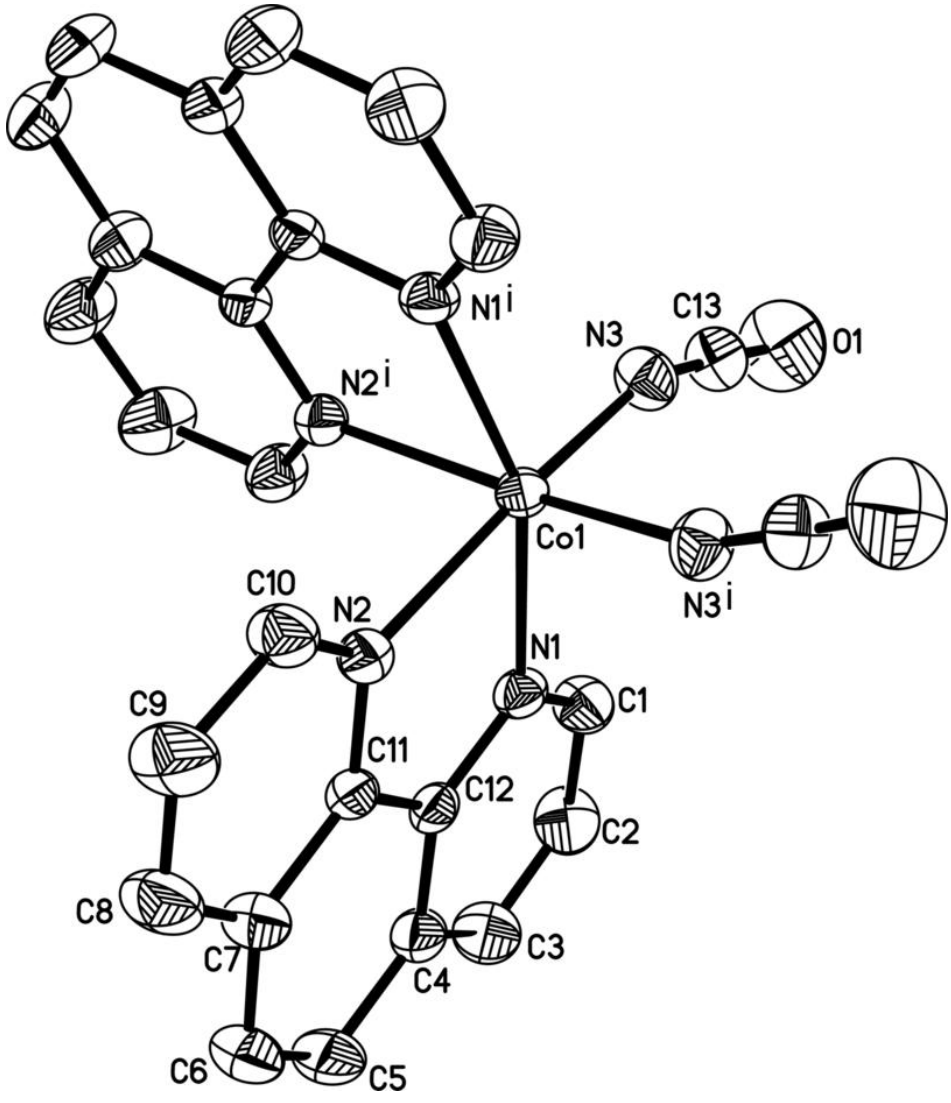
Geometric parameters (Å, °)

Co1—N1	2.168 (2)	C4—C12	1.403 (4)

Co1—N2	2.223 (3)	C4—C5	1.430 (5)
Co1—N3	2.058 (3)	C5—C6	1.360 (6)
O1—C13	1.220 (4)	C5—H5	0.9300
N1—C1	1.321 (5)	C6—C7	1.420 (5)
N1—C12	1.359 (4)	C6—H6	0.9300
N2—C10	1.322 (4)	C7—C8	1.394 (5)
N2—C11	1.354 (4)	C7—C11	1.418 (5)
N3—C13	1.133 (4)	C8—C9	1.365 (6)
C1—C2	1.393 (5)	C8—H8	0.9300
C1—H1	0.9300	C9—C10	1.414 (5)
C2—C3	1.374 (6)	C9—H9	0.9300
C2—H2	0.9300	C10—H10	0.9300
C3—C4	1.399 (5)	C11—C12	1.430 (4)
C3—H3	0.9300		
$N3^{i}$—Co1—N3	98.13 (17)	C4—C3—H3	120.1
$N3^{i}$—Co1—N1	100.52 (11)	C3—C4—C12	117.5 (3)
N3—Co1—N1	93.64 (11)	C3—C4—C5	123.8 (3)
$N3^{i}$—Co1—$N1^{i}$	93.64 (11)	C12—C4—C5	118.7 (3)
N3—Co1—$N1^{i}$	100.52 (11)	C6—C5—C4	121.7 (3)
N1—Co1—$N1^{i}$	158.36 (13)	C6—C5—H5	119.2
$N3^{i}$—Co1—N2	88.23 (11)	C4—C5—H5	119.2
N3—Co1—N2	168.55 (10)	C5—C6—C7	120.4 (4)
N1—Co1—N2	75.76 (9)	C5—C6—H6	119.8
$N1^{i}$—Co1—N2	88.51 (9)	C7—C6—H6	119.8
$N3^{i}$—Co1—$N2^{i}$	168.55 (10)	C8—C7—C11	117.1 (3)
N3—Co1—$N2^{i}$	88.23 (11)	C8—C7—C6	123.3 (3)
N1—Co1—$N2^{i}$	88.51 (9)	C11—C7—C6	119.5 (4)
$N1^{i}$—Co1—$N2^{i}$	75.76 (9)	C9—C8—C7	120.7 (4)
N2—Co1—$N2^{i}$	87.17 (13)	C9—C8—H8	119.6
C1—N1—C12	118.3 (3)	C7—C8—H8	119.6
C1—N1—Co1	126.2 (2)	C8—C9—C10	118.2 (4)
C12—N1—Co1	115.26 (19)	C8—C9—H9	120.9
C10—N2—C11	118.5 (3)	C10—C9—H9	120.9
C10—N2—Co1	128.2 (2)	N2—C10—C9	123.0 (3)
C11—N2—Co1	113.28 (19)	N2—C10—H10	118.5
C13—N3—Co1	160.3 (3)	C9—C10—H10	118.5
N1—C1—C2	123.2 (3)	N2—C11—C7	122.4 (3)
N1—C1—H1	118.4	N2—C11—C12	118.1 (3)
C2—C1—H1	118.4	C7—C11—C12	119.5 (3)
C3—C2—C1	118.7 (4)	N1—C12—C4	122.4 (3)
C3—C2—H2	120.6	N1—C12—C11	117.5 (2)
C1—C2—H2	120.6	C4—C12—C11	120.1 (3)
C2—C3—C4	119.8 (3)	N3—C13—O1	175.3 (4)
C2—C3—H3	120.1		

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

Fig. 1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C1
C11
C12
C2
C8
C7
C4
C3
C6
C5