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

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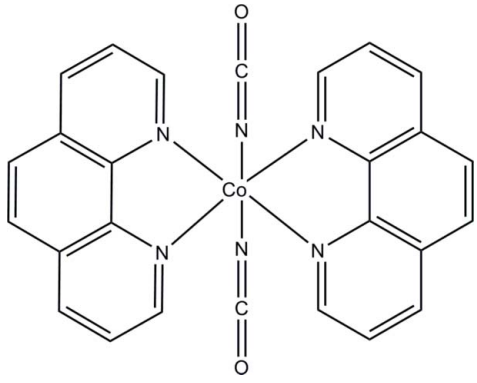
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.044; $wR$ factor = 0.144; data-to-parameter ratio = 11.9.

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
$\mu$ = 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).

## References

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# supporting information

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

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

**Dao-Peng Zhang, Nai-Chang Tian and Xiao-Mei Zhang**

### S1. 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).

### S2. 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%.

### S3. Refinement

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

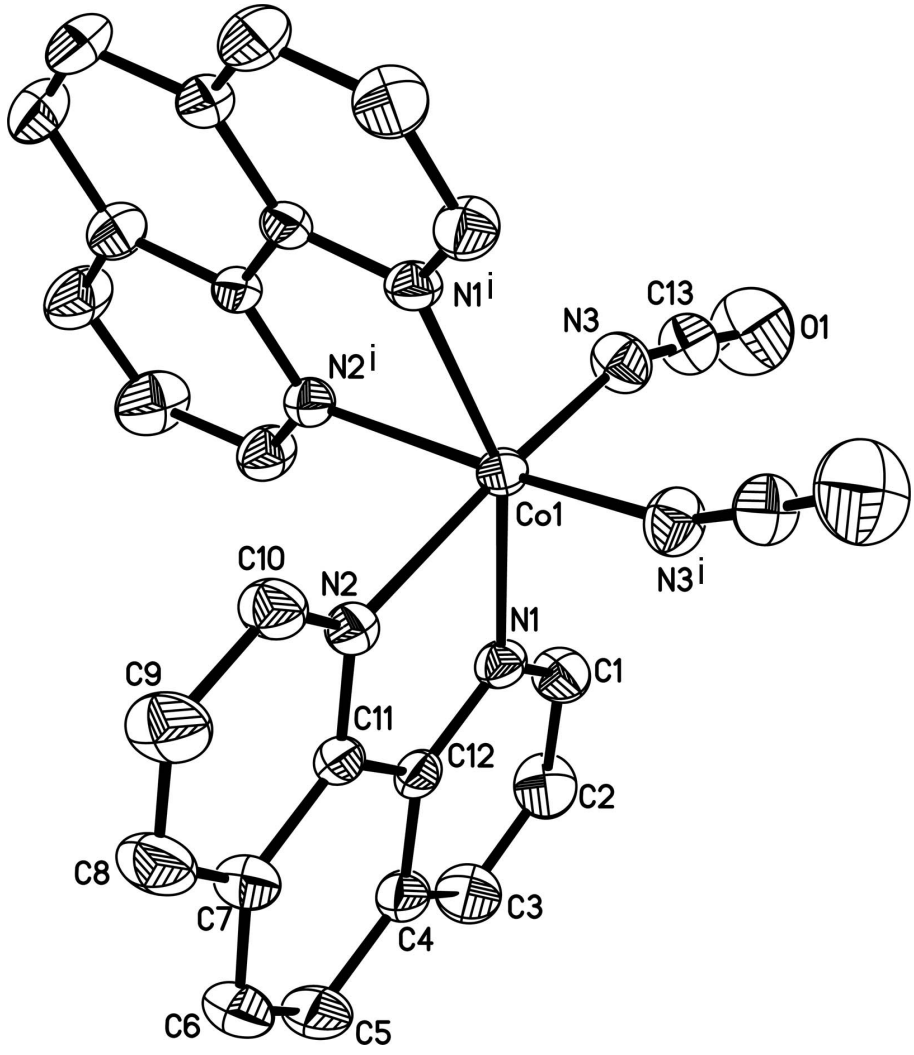


**Figure 1**

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

*Crystal data*

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

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
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
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.4°
$h$ = −15→15
$k$ = −7→11
$l$ = −19→19

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.144
$S$ = 1.06
1890 reflections
159 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0851P)^2 + 1.8714P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.70 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.62 e Å$^{-3}$

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

| | *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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

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