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

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The title compound, $[Co(NCS)_2(C_{10}H_8N_2)_2]$, is isostructural with the Fe^{II} analogue. The Co^{II} atom lies on a crystallographic twofold axis and the thiocyanate ligands adopt a *cis* configuration.

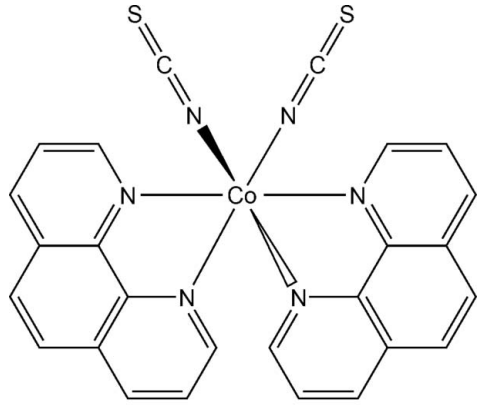
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.111
Data-to-parameter ratio = 16.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The title compound, $[Co(NCS)_2(C_{10}H_8N_2)_2]$, is isostructural with its Fe^{II} analogue (Gallois *et al.*, 1990). In the crystal structure, the molecule is positioned on a crystallographic twofold axis, with the Co^{II} atom lying in a distorted octahedral coordination environment (Fig. 1). The planes through the two 1,10-phenanthroline ligands are approximately perpendicular to each other [dihedral angle 87.6 (1)°] and the thiocyanate ligands adopt a *cis* configuration. The two Co—N distances to each bidentate phenthroline ligand are closely comparable [2.1740 (17) and 2.1642 (15) Å], while the Co—N distance to the thiocyanate ligand is significantly shorter [2.0597 (18) Å].



(I)

Experimental

Single crystals of the title compound were obtained at the interface of a layered system, with the lower layer comprising an aqueous solution (3 ml) of cobalt(II) nitrate (0.1 mmol) and potassium thiocyanate (0.1 mmol), and the upper layer comprising a methanolic solution (0.3 ml) of 1,10-phenanthroline (0.1 mmol).

Crystal data

$[Co(NCS)_2(C_{10}H_8N_2)_2]$
M_r = 535.50
Orthorhombic, *Pbcn*
a = 13.153 (3) Å
b = 10.078 (2) Å
c = 17.489 (4) Å
V = 2318.4 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.95 mm^{-1}
T = 293 (2) K
0.25 × 0.20 × 0.20 mm

Data collection

Rigaku Mercury70 CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)
T_{min} = 0.775, T_{max} = 0.827
16718 measured reflections
2664 independent reflections
2400 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.111
S = 1.03
2664 reflections
159 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co—N3	2.0597 (18)	Co—N1	2.1740 (17)
Co—N2	2.1642 (15)		
N3—Co—N3^{i}	94.25 (11)	N3^{i}—Co—N1	88.57 (8)
N3—Co—N2	92.21 (7)	N2—Co—N1	76.55 (6)
N3^{i}—Co—N2	99.54 (7)	N2^{i}—Co—N1	91.25 (6)
N2—Co—N2^{i}	162.73 (9)	N1—Co—N1^{i}	90.78 (9)
N3—Co—N1	168.72 (6)		

Symmetry code: (i) $-x, y, -z+\frac{3}{2}$.

H atoms were included in calculated positions, with C—H = 0.93 Å, and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1999); software used to prepare material for publication: *SHELXTL/PC*.

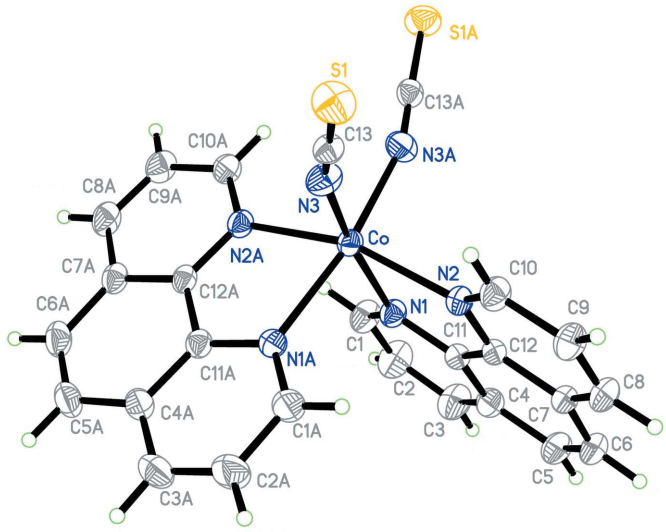


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level. Atoms with the suffix A are generated by the symmetry operator $(-x, y, \frac{3}{2}-z)$.

References

Gallois, B., Real, J. A., Hauw, C. & Zarembowitch, J. (1990). *Inorg. Chem.* **29**, 1152–1158.
Rigaku (2000). *CrystalClear*. Version 1.3.6. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1999). *SHELXTL/PC*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.