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# *trans*-Bis(1,4-butanediamine)bis(isothiocyanato)-cobalt(III) thiocyanate

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**Key indicators**

Single-crystal X-ray study
*T* = 296 K
Mean σ(C–C) = 0.004 Å
*R* factor = 0.033
*wR* factor = 0.094
Data-to-parameter ratio = 27.0

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



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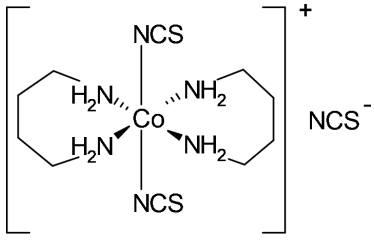
The title compound, $[Co(NCS)_2(C_4H_{12}N_2)_2]NCS$, (I), has an octahedral coordination geometry, in which one of the seven-membered chelate rings adopts the chair form and the other the twist-boat form.

## Comment

Metal complexes of 1,4-butanediamine, also known as putrescin or tetramethylenediamine (tmd), are of interest in the context of bioinorganic chemistry (Gasowska *et al.*, 2000). Only a few structures have been reported for transition metal complexes of tmd (Sato *et al.*, 1974; Shimoi *et al.*, 1988; Kurachi & Ohba, 1992).




(I)

The two geometrical isomers of $[Co^{III}(NCS)_2(tmd)_2]^+$ have been prepared and their geometrical configurations have been determined from their spectroscopic properties (Nagata & Kanamori, 2001). The present X-ray analysis confirms the *trans* configuration for one of the isomers, (I) (Fig. 1). In (I), the two seven-membered chelate rings adopt different conformations (Fig. 2). The conformation of Fig. 2(*a*) corresponds to the chair form that has been found in *trans*-$[Co(III)(NO_2)_2(tmd)_2]^+$ (Shimoi *et al.*, 1988). The other chelate ring (Fig. 2*b*) adopts approximately the twist-boat form. The coordination bond distances and angles are in the normal ranges.

## Experimental

The title compound, (I), was prepared by adapting the procedures described by Nagata *et al.* (1985) and Nagata & Kanamori (2001). Crystals of (I) were obtained by evaporation of an aqueous solution at room temperature.

*Crystal data*

$[Co(NCS)_2(C_4H_{12}N_2)_2]NCS$
$M_r$ = 409.48
Monoclinic, $P2_1/c$
$a$ = 9.739 (2) Å
$b$ = 13.647 (4) Å
$c$ = 14.5479 (19) Å
$\beta$ = 107.790 (13)°
$V$ = 1841.2 (7) Å$^3$
$Z$ = 4
$D_x$ = 1.477 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta$ = 14.8–15.0°
$\mu$ = 1.28 mm$^{-1}$
$T$ = 296 (2) K
Prism, brown
0.20 × 0.20 × 0.15 mm

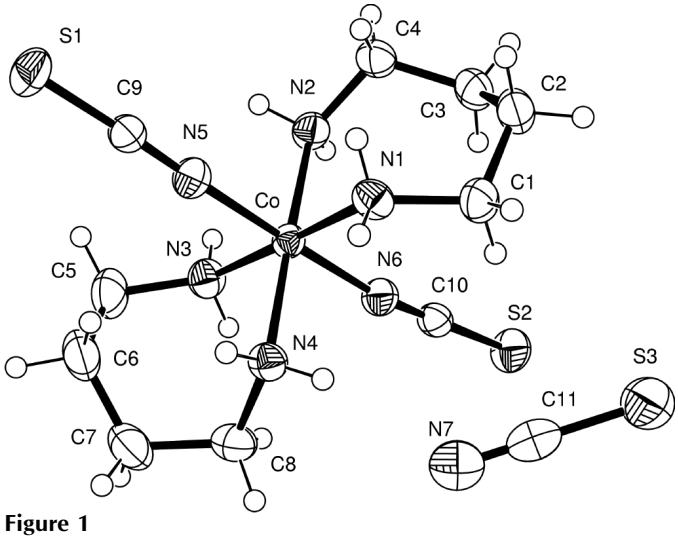



**Figure 1**
The molecular structure of (I) showing the labelling of the non-H atoms. Displacement ellipsoids are shown at 50% probability levels.

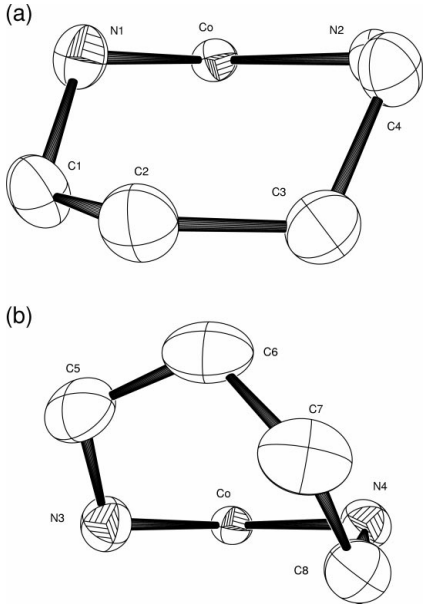



**Figure 2**
The conformations of the chelate rings projected along the bisector of the N—Co—N angle.

*Data collection*

Rigaku AFC-7*R* diffractometer
$\omega$–$2\theta$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.784, $T_{max}$ = 0.831
5653 measured reflections
5371 independent reflections
4027 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027
$\theta_{max}$ = 30.0°
$h = 0 \rightarrow 13$
$k = 0 \rightarrow 19$
$l = -20 \rightarrow 19$
3 standard reflections
frequency: 60 min
intensity decay: 1.8%

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.094
$S$ = 1.06
5371 reflections
199 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0409P)^2 + 0.8638P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.56 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Co—N1 | 1.9881 (17) | Co—N4 | 1.9930 (17) |
| Co—N2 | 1.9747 (17) | Co—N5 | 1.8918 (17) |
| Co—N3 | 1.9856 (17) | Co—N6 | 1.8961 (17) |
| | | | |
| N1—Co—N2 | 92.21 (7) | N2—Co—N6 | 89.10 (7) |
| N1—Co—N3 | 177.26 (7) | N3—Co—N4 | 90.44 (7) |
| N1—Co—N4 | 88.51 (7) | N3—Co—N5 | 92.13 (8) |
| N1—Co—N5 | 85.41 (8) | N3—Co—N6 | 87.45 (8) |
| N1—Co—N6 | 95.05 (7) | N4—Co—N5 | 93.29 (8) |
| N2—Co—N3 | 88.94 (7) | N4—Co—N6 | 88.60 (7) |
| N2—Co—N4 | 177.64 (7) | N5—Co—N6 | 178.07 (8) |
| N2—Co—N5 | 89.01 (8) | | |

H atoms bonded to C and N atoms were placed geometrically and refined using a riding model *via* the *SHELXL*97 *HFIX*/*AFIX* 23 facility. The displacement parameter was set as 1.2 times that of the parent atom.

Data collection: *AFC*-7*R Diffractometer Control Software* (Rigaku, 1999); cell refinement: *AFC*-7*R Diffractometer Control Software;* data reduction: *AFC*-7*R Diffractometer Control Software*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

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