Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tris(ethyldithiocarbamato-κ^2S,S')cobalt(III)

Gui-Ling Zhang, Yan-Tuan Li* and Zhi-Yong Wu

Marine Drug and Food Institute, Ocean University of China, 266003 Qingdao, People's Republic of China

Correspondence e-mail: yantuanli@ouc.edu.cn

Received 5 January 2006
Accepted 18 January 2006

Key indicators

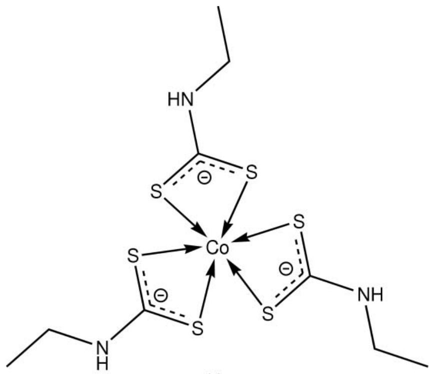
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.010 Å
R factor = 0.053
wR factor = 0.189
Data-to-parameter ratio = 17.4

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

In the crystal structure of the title compound, $[Co(C_3H_6NS_3)_3]$, the Co^{II} atom lies on a threefold axis; its coordination geometry is distorted octahedral, consisting of six S atoms from three chelating ethyldithiocarbamate ligands.

Comment

Studies on dithiocarbamic acids have been carried out for many years. Transition metal complexes of *N*,*N*-dialkyldithiocarbamates (R_2NCS_2) and related dithio ligands are of interest because of their resemblance to the active centers of metal–sulfur proteins that mediate redox reactions and electron transfer in biological systems (Burns *et al.*, 1980; Enemark *et al.*, 1993; Rees *et al.*, 1993). While there are numerous examples of tris(dialkyldithiocarbamato)metal complexes, monoalkyldithiocarbamate and its complexes are relatively scarce (Newman & White, 1972; Raston & White, 1974; Christidis & Rentzeperis, 1979; Kamenicek *et al.*, 1990).



(I)

In the crystal structure of the title compound, (I), the Co^{II} atom lies on a threefold axis (Fig. 1). The coordination of the Co^{II} atom is distorted octahedral, consisting of six S atoms from three chelating ethyldithiocarbamate ligands, and is similar to that of tris(dialkyldithiocarbamato)metal complexes (Jian *et al.*, 2002; Mohamed *et al.*, 2003). The CoS_2CN fragments are each nearly planar, the two planes being inclined at 83.55 (9)°.

Experimental

Carbon disulfide (25.2 g, 0.33 mol) was added dropwise to a solution of α-alanine (23.5 g, 0.33 mol) and potassium hydroxide (37.0 g, 0.66 mol) in 95% ethanol at 273 K. Mixing was carried out with constant stirring with a magnetic stirrer. The intended compound was potassium 2-dithioformylpropanoate (Tarafder *et al.*, 2001), but decarboxylation of the product occurred to yield potassium ethyldithiocarbamate was obtained. An ethanol solution of the potassium salt of the ligand (0.6 mmol) was added dropwise to cobalt(III) chloride (0.2 mmol) in ethanol. After the small amount of insoluble material was removed, the resulting red solution was allowed to evaporate at room temperature, affording red brown crystals after two weeks.

Crystal data

$[Co(C_3H_6NS_2)_3]$
$M_r = 419.55$
Trigonal, $R\overline{3}$
$a = 14.891$ (2) Å
$c = 13.296$ (3) Å
$V = 2553.5$ (6) Å^3
$Z = 6$
$D_x = 1.637$ Mg m^{-3}

Mo *Kα* radiation
Cell parameters from 1029 reflections
$\theta = 2.2$–25.2°
$\mu = 1.73$ mm^{-1}
$T = 293$ (2) K
Block, brown
0.45 × 0.18 × 0.14 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.509$, $T_{max} = 0.793$
4247 measured reflections

1029 independent reflections
840 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 25.2°$
$h = -17 \rightarrow 17$
$k = -15 \rightarrow 17$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.189$
$S = 1.20$
1029 reflections
59 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1154P)^2 + 3.3736P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.17$ e Å^{-3}
$\Delta\rho_{min} = -0.98$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—S1	2.2773 (14)	N1—C1	1.320 (7)
Co1—S2	2.2820 (14)	N1—C2	1.473 (6)
S1—C1	1.689 (5)	C2—C3	1.501 (9)
S2—C1	1.686 (5)		
S1—Co1—S1^{i}	94.07 (5)	S2—Co1—S2^{i}	94.31 (6)
S1—Co1—S2	76.56 (5)	C1—S1—Co1	84.94 (18)
S1—Co1—S2^{i}	96.60 (5)	C1—S2—Co1	84.85 (19)
S1—Co1—S2^{ii}	166.24 (5)		
C2—N1—C1—S2	6.3 (7)	C1—N1—C2—C3	−162.9 (5)
C2—N1—C1—S1	−175.2 (4)		

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

All H atoms were placed in calculated positions, with C—H distances of 0.97 (CH_2) or 0.96 Å (CH_3) and N—H distances of 0.86 Å, and were included in the final cycles of refinement as riding, with U_{iso}(H) values of $1.2U_{eq}$(N and methylene C) or $1.5U_{eq}$(methyl C). The highest peak and deepest hole in the final difference map were about 1 Å from atom Co1.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

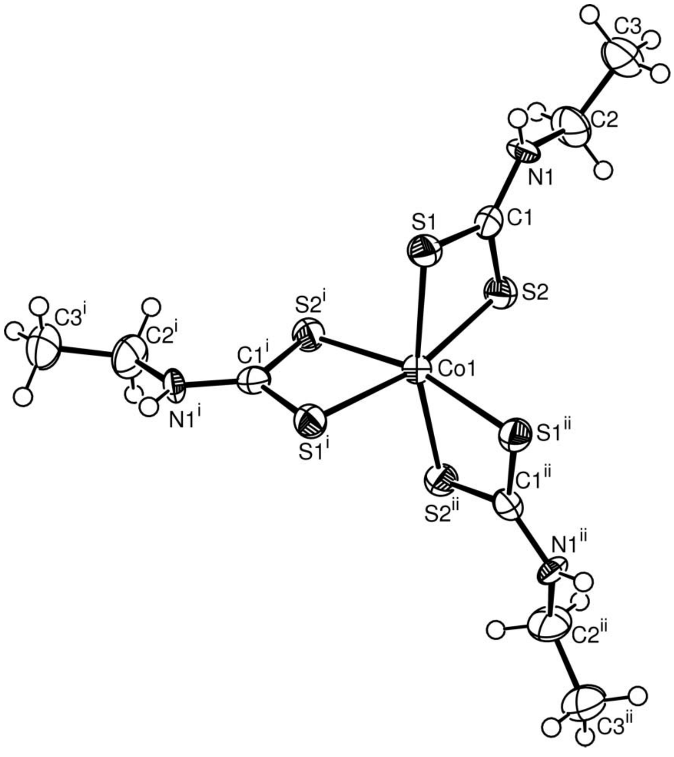


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids. [Symmetry codes: (i) $1-y, x-y, z$, (ii) $y-x+1, 1-x, z$.]

This project was supported by the National Natural Science Foundation of China (No. 20471056).

References

Bruker (2002). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Burns, R. P., McCullough, F. P. & McAuliffe, C. A. (1980). *Adv. Inorg. Nucl. Chem.* **23**, 211–213.
Christidis, P. C. & Rentzeperis, P. J. (1979). *Acta Cryst.* B**35**, 2543–2547.
Enemark, J. H. & Young, C. G. (1993). *Adv. Inorg. Chem.* **40**, 1–4.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Jian, F.-F., Bei, F.-L, Zhao, P.-S., Wang, X., Fun, H.-K. & Chinnakali, K. (2002). *J. Coord. Chem.* **55**, 429–437.
Kamenicek, J., Pastorek, R., Brezina, F., Kratochvil, B. & Travnicek, Z. (1990). *Collect. Czech. Chem. Commun.* **55**, 1010–1013.
Mohamed, A. K., Auner, N. & Bolte, M. (2003). *Acta Cryst.* E**59**, m188–m189.
Newman, P. W. G. & White, A. H. (1972). *J. Chem. Soc. Dalton Trans.* pp. 1460–1464.
Raston, C. L. & White, A. H. (1974). *J. Chem. Soc. Dalton Trans.* pp. 1790–1792.
Rees, D. C., Chan, M. K. & Kim, J. (1993). *Adv. Inorg. Chem.* **40**, 89–93.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Tarafder, M. T. H., Ali, A. M., Wong, Y. W., Wong, S. H. & Crouse, K. A. (2001). *Synth. React. Inorg. Met.-Org. Chem.* **31**, 115–125.

Acta Cryst. (2006). E**62**, m350–m351 Zhang *et al.* • $[Co(C_3H_6NS_2)_3]$ **m351**