Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Dichlorobis(3,4,5,6-tetrahydropyrimidinium-2-thiolato-*S*)cobalt(II)

Ibrahim Abdul Razak,[a] Anwar Usman,[a] Hoong-Kun Fun,[a]* Bohari M. Yamin[b] and Wooi Keat Goh[b]

[a]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and [b]School of Chemical Sciences and Food Technology, Universiti Kebangsaan Malaysia, 43600 Bangi, Selangor, Malaysia

Correspondence e-mail: hkfun@usm.my

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.051
wR factor = 0.142
Data-to-parameter ratio = 21.9

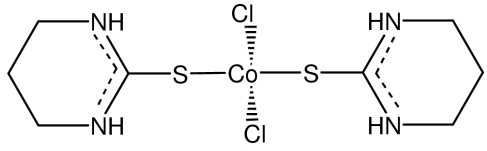
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 28 September 2001
Accepted 9 October 2001
Online 13 October 2001

In the title compound, $[CoCl_2(C_4H_8N_2S)_2]$, the coordination around the Co atom is slightly distorted tetrahedral, with an average angle of 109.46 (4)°. Intermolecular interactions between the N and Cl atoms result in interconnected two-dimensional molecular network ribbons throughout the structure.

Comment

Continuing our interest in the diverse complexing behaviour of cobalt complexes with monothione ligands, a crystal of the title compound, (I), has been studied. Earlier work has shown that 1-methylimidazolidine-2(3*H*)-thione (meimt) gives rise to complexes with the molecular formula $Co(meimt)_4(NO_3)_2\cdot H_2O$ in ethanol solvent and $Co(meimt)_2(NO_3)_2$ in ethyl acetate solvent (Raper & Nowell, 1980); a perchlorate has also been reported, *viz*. $[Co(meimt)_4](ClO_4)_2$ (Raper & Nowell, 1979).



(I)

The bond lengths and angles of the ligands in (I) are comparable with those reported for dichlorotetrakis(trimethylenethiourea)nickel(II) (Luth & Truter, 1968). The Co atom is tetrahedrally coordinated by two Cl atoms and two S atoms (Fig. 1). The angles around the Co atom are in the range 97.45 (3)–117.17 (4)°, with an average of 109.46 (4)°, implying that the tetrahedron is slightly distorted.

In the crystal, all the N atoms are involved in intramolecular and intermolecular interactions with the Cl atoms. Atoms N1 and N4 form intramolecular interactions, whereas atoms N3 and N2 form intermolecular interactions. The intermolecular interactions between N2 and Cl2(x, $1+y$, z) form molecular ribbons along the *b* axis, stacking along the *a* axis (Fig. 2). The other intermolecular interactions between N3 and Cl2(x, $1-y$, $\frac{1}{2}+z$) interconnect these ribbons into a two-dimensional molecular network throughout the structure.

Experimental

2.4 g of propylenethiourea (20 mmol) was added to a solution of cobalt(II) chloride (1.3 g, 10 mmol) in acetonitrile (20 ml). The mixture was stirred at ambient temperature for 30 min. After stirring, the solution was poured into crystal dishes and covered with alumi-

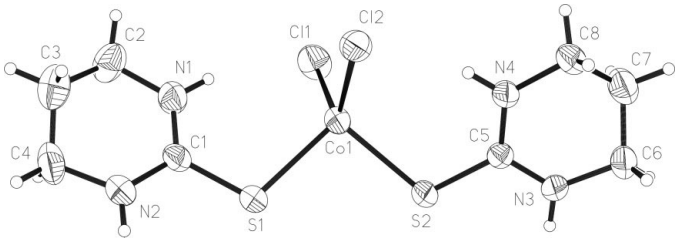


Figure 1
The structure of the title compound showing 50% probability displacement ellipsoids and the atom-numbering scheme.

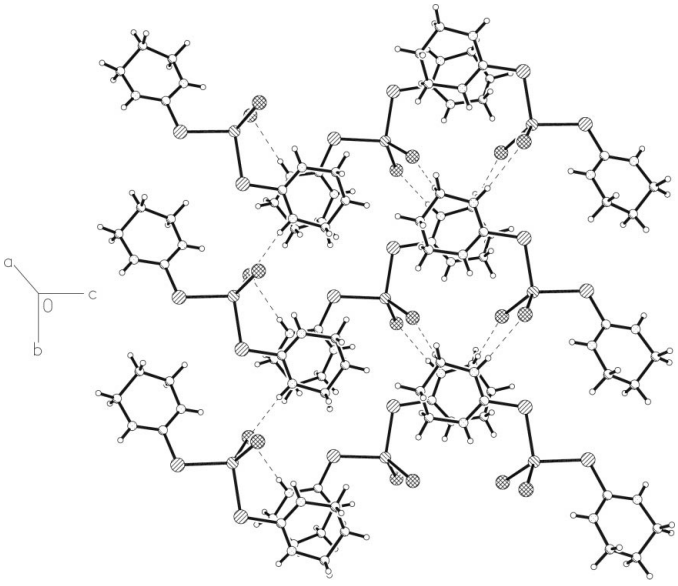


Figure 2
Packing diagram of the two-dimensional network, viewed down the *a* axis

nium foil to allow the solvent to evaporate. After a few weeks, blue crystals were obtained; these were washed with hexane and, after drying, a suitable single-crystal was selected for X-ray structure determination.

Crystal data

$[CoCl_2(C_4H_8N_2S)_2]$
M_r = 362.20
Monoclinic, *C*2/*c*
a = 32.0245 (14) Å
b = 7.1329 (3) Å
c = 14.6141 (6) Å
β = 116.864 (1)°
V = 2978.0 (2) Å^3
Z = 8
D_x = 1.616 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 7650 reflections
θ = 1.4–29.5°
μ = 1.78 mm^{-1}
T = 293 (2) K
Slab, blue
0.46 × 0.24 × 0.16 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
T_{min} = 0.496, T_{max} = 0.764
9648 measured reflections
3397 independent reflections
2635 reflections with $I > 2\sigma(I)$
R_{int} = 0.089
θ_{max} = 27.5°
h = −36 → 41
k = −8 → 9
l = −18 → 18

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.142
S = 0.98
3397 reflections
155 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0748P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −1.03 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0033 (4)

Table 1
Selected geometric parameters (Å, °).

Co1—Cl1	2.230 (1)	N2—C4	1.468 (5)
Co1—Cl2	2.282 (1)	N3—C5	1.315 (4)
Co1—S1	2.313 (1)	N3—C6	1.463 (4)
Co1—S2	2.319 (1)	N4—C5	1.322 (3)
S1—C1	1.734 (3)	N4—C8	1.456 (4)
S2—C5	1.726 (3)	C2—C3	1.483 (6)
N1—C1	1.312 (4)	C3—C4	1.498 (6)
N1—C2	1.470 (4)	C6—C7	1.512 (5)
N2—C1	1.320 (4)	C7—C8	1.494 (5)
Cl1—Co1—Cl2	107.97 (4)	Cl1—Co1—S2	117.17 (4)
Cl1—Co1—S1	110.43 (4)	Cl2—Co1—S2	110.17 (3)
Cl2—Co1—S1	113.55 (4)	S1—Co1—S2	97.45 (3)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*A*···Cl2	0.86	2.45	3.263 (3)	158
N1—H1*A*···Cl1	0.86	2.53	3.358 (3)	161
N2—H2*A*···Cl2^{i}	0.86	2.64	3.483 (3)	167
N3—H3*A*···Cl2^{ii}	0.86	2.50	3.353 (3)	171

Symmetry codes: (i) $x, 1+y, z$; (ii) $x, 1-y, \frac{1}{2}+z$.

After checking their presence in a difference map, all the H atoms were geometrically fixed and allowed to ride on their attached atoms.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL, PARST* (Nardelli, 1995) and *PLATON* (Spek, 1990).

The authors would like to thank the Malaysian Government, Universiti Sains Malaysia and Universiti Kebangsaan Malaysia for research grants No. 305/PFIZIK/610961 and 09-02-02-0163, respectively. AU thanks the Universiti Sains Malaysia for a Visiting Postdoctoral Fellowship.

References

Luth, H. & Truter, M. R. (1968). *J. Chem. Soc. A*, pp. 1879–1886.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Raper, E. S. & Nowell, I. W. (1979). *Acta Cryst.* B**35**, 1600.
Raper, E. S. & Nowell, I. W. (1980). *Inorg. Chim. Acta*, **43**, 165–172.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Spek, A. L. (1990). *Acta Cryst.* A**46**, C-34.