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trans-Dichlorobis[pyrimidine-2(1*H*)-thione-κ*N*]-cobalt(II)

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Key indicators

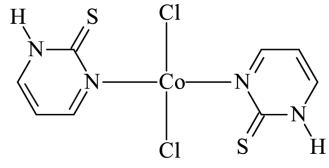
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.026
wR factor = 0.071
Data-to-parameter ratio = 16.1

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

In the title complex, $[CoCl_2(C_4H_4N_2S)_2]$, the pyrimidine-2(1*H*)-thione ligand coordinates through nitrogen to the Co^{II} atom, which possesses tetrahedral geometry. The molecule lies on a twofold rotation axis.

Comment

In our earlier work, heterocyclic thiones were used for studying the binding properties with a soft Lewis acid such as Cu^{I}. We found that heterocyclic thiones coordinate in a monodentate fashion through the S atom (Li, Luo *et al.*, 2004; Li, Shi *et al.*, 2004). In this work, the ligand coordinates to the Co^{II} ion in a monodentate manner through an endocyclic N atom rather than the exocyclic S atom, giving the title complex, (I).



(I)

In (I) (Fig. 1), the Co atom, on a twofold axis, is coordinated by two Cl atoms and two N atoms from two pyrimidinethione ligands in a distorted tetrahedral geometry. The Co—N and Co—Cl bond lengths are comparable to values found in the literature (Atherton *et al.*, 1999; Mihalcik *et al.*, 2004). The crystal structure is stabilized by an N—H···Cl hydrogen bond (Table 2 and Fig. 2).

Experimental

Solid cobalt dichloride hexahydrate (0.0070 g, 0.03 mmol) and 2-mercaptopyrimidine (0.0066 g, 0.06 mmol) were carefully added to CH_2Cl_2/CH_3CN (3:2). This solution was stirred for 30 min and left for one week. Dark-blue block-like crystals were obtained (yield 80%).

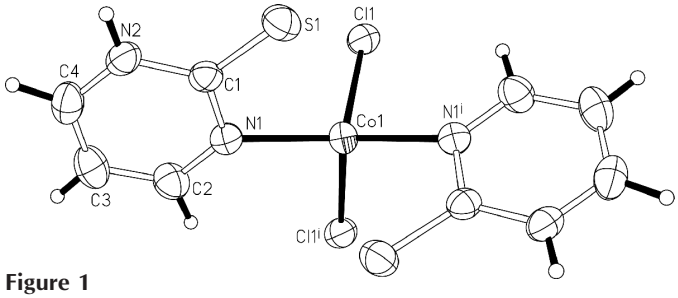


Figure 1
*ORTEP*II (Johnson, 1976) plot of the molecule of (I) with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.[Symmetry code: (i) $1-x, y, \frac{3}{2}-z$.]

Crystal data

$[CoCl_2(C_4H_4N_2S)_2]$
M_r = 354.13
Monoclinic, $C2/c$
a = 12.3690 (8) Å
b = 8.3050 (6) Å
c = 13.9204 (9) Å
β = 115.013 (1)°
V = 1295.9 (2) Å^3
Z = 4
D_x = 1.815 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2946 reflections
θ = 3.1–27.7°
μ = 2.04 mm^{-1}
T = 295 (2) K
Block, blue
0.18 × 0.14 × 0.12 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.645, T_{max} = 0.792
5449 measured reflections
1518 independent reflections
1417 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 27.8°
$h = -15 \rightarrow 16$
$k = -10 \rightarrow 10$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.071
S = 1.05
1518 reflections
94 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0464P)^2 + 0.3426P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—N1	2.045 (1)	Co1—Cl1	2.3540 (5)
N1—Co1—N1^{i}	141.41 (8)	N1—Co1—Cl1^{i}	97.58 (4)
N1—Co1—Cl1	107.57 (4)	Cl1—Co1—Cl1^{i}	97.95 (2)

Symmetry code: (i) $1-x, y, \frac{3}{2}-z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2n···Cl1^{ii}	0.85 (1)	2.26 (1)	3.088 (2)	164 (2)

Symmetry code: (ii) $\frac{1}{2}-x, \frac{3}{2}-y, 1-z$.

H atoms were located in a difference map and refined isotropically.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

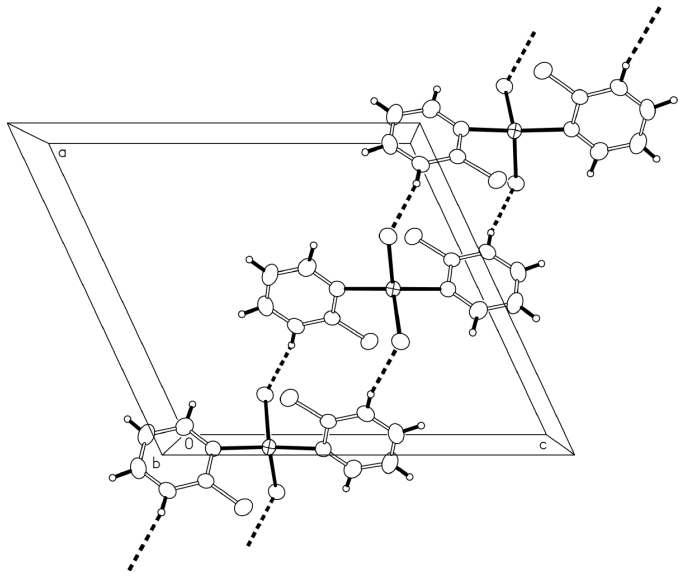


Figure 2
Packing diagram showing the hydrogen bonds as dashed lines. The view is on to the *ac* plane.

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