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Key indicators

Single-crystal X-ray study
T = 298 K
Mean $\sigma(\text{C}-\text{C}) = 0.010 \text{ \AA}$
R factor = 0.061
wR factor = 0.192
Data-to-parameter ratio = 14.5

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

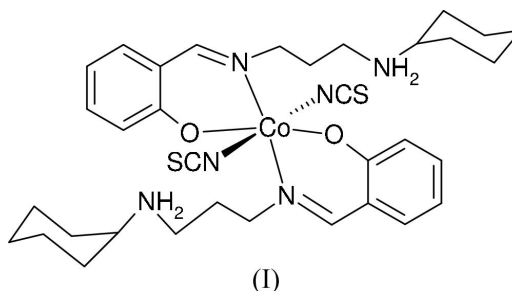
Bis{2-[3-(cyclohexylammonio)propylimino-methyl]phenolato}dithiocyanatocobalt(II)

The title Schiff base compound, $[\text{Co}(\text{C}_{16}\text{H}_{24}\text{N}_2\text{O})_2(\text{NCS})_2]$, is centrosymmetric with the octahedrally coordinated Co^{II} atom lying on an inversion center. The Co atom is coordinated by two N atoms and two O atoms from two 2-[(3-cyclohexylaminopropylimino)methyl]phenolate Schiff base ligands and another two N atoms from two thiocyanate anions. In the crystal structure, the molecules are linked by $\text{N}-\text{H}\cdots\text{S}$ intermolecular hydrogen bonds, forming a polymer extending in the *b*-axis direction.

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Comment

Cobalt complexes are of great interest in coordination chemistry in relation to catalysis and enzymatic reactions, magnetism and molecular architectures (Billson *et al.*, 2000; Kotera *et al.*, 2003; Fritsky *et al.*, 2003). As an extension of work on the structural characterization of cobalt complexes, the title mononuclear cobalt(II) complex, (I), is reported here.



Compound (I) is an electronically neutral mononuclear centrosymmetric cobalt(II) compound (Fig. 1), which is isostructural with the copper(II) complex reported by Nie (2004). The Co^{II} atom has an octahedral geometry and is six-coordinated by two Schiff base ligands and two thiocyanate anions. The Schiff base acts as a bidentate ligand and chelates to atom Co1 through the O atom and imine N atom. The thiocyanate ligands are monodentate and coordinate to atom Co1 via the N atoms. All the bond lengths and angles are in normal ranges (Table 1). As expected, the cyclohexyl group adopts a chair conformation to minimize steric effects.

In the crystal structure, the molecules are linked by $\text{N}-\text{H}\cdots\text{S}$ hydrogen bonds, forming a polymer chain extending in the *b*-axis direction (see Table 2 and Fig. 2).

Experimental

Salicylaldehyde (0.1 mmol, 12.2 mg), *N*-cyclohexylpropane-1,3-diamine (0.1 mmol, 15.7 mg), ammonium thiocyanate (0.2 mmol, 15.2 mg) and $\text{Co}(\text{CH}_3\text{COO})_2\cdot 4\text{H}_2\text{O}$ (0.1 mmol, 24.9 mg) were

dissolved in methanol (15 ml). The mixture was stirred at room temperature for 1 h to give a clear brown solution. After keeping the solution in air for 12 d, brown block-shaped crystals were formed.

Crystal data

$[\text{Co}(\text{C}_{16}\text{H}_{24}\text{N}_2\text{O})_2(\text{NCS})_2]$	$D_x = 1.317 \text{ Mg m}^{-3}$
$M_r = 695.83$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 755 reflections
$a = 10.912 (7) \text{ \AA}$	$\theta = 2.8\text{--}23.4^\circ$
$b = 7.797 (5) \text{ \AA}$	$\mu = 0.65 \text{ mm}^{-1}$
$c = 20.777 (13) \text{ \AA}$	$T = 298 (2) \text{ K}$
$\beta = 96.899 (13)^\circ$	Block, brown
$V = 1754.9 (19) \text{ \AA}^3$	$0.29 \times 0.17 \times 0.11 \text{ mm}$
$Z = 2$	

Data collection

Bruker SMART CCD area-detector diffractometer	2975 independent reflections
ω scans	1337 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.101$
$T_{\text{min}} = 0.835$, $T_{\text{max}} = 0.932$	$\theta_{\text{max}} = 25.0^\circ$
7131 measured reflections	$h = -10 \rightarrow 12$
	$k = -9 \rightarrow 7$
	$l = -12 \rightarrow 24$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.061$	$w = 1/[\sigma^2(F_o^2) + (0.0889P)^2]$
$wR(F^2) = 0.192$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.84$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2975 reflections	$\Delta\rho_{\text{max}} = 0.54 \text{ e \AA}^{-3}$
205 parameters	$\Delta\rho_{\text{min}} = -0.55 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

Co1—O1	2.031 (4)	Co1—N3	2.127 (6)
Co1—N1	2.087 (5)		
O1—Co1—O1 ⁱ	180	N1—Co1—N3 ⁱ	92.9 (2)
O1—Co1—N1 ⁱ	91.3 (2)	O1—Co1—N3	88.7 (2)
O1—Co1—N1	88.7 (2)	N1—Co1—N3	87.1 (2)
N1 ⁱ —Co1—N1	180	N3 ⁱ —Co1—N3	180
O1—Co1—N3 ⁱ	91.3 (2)		

Symmetry code: (i) $-x, 1 - y, -z$.

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
N2—H2B \cdots O1 ⁱ	0.90	1.78	2.682 (6)	175
N2—H2A \cdots S1 ⁱⁱ	0.90	2.44	3.336 (6)	173

Symmetry codes: (i) $-x, 1 - y, -z$; (ii) $-x, 2 - y, -z$.

The ratio of observed to unique reflections is low (45%), probably because of the poor diffraction quality of the crystal. All the H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with distances $\text{C--H} = 0.93\text{--}0.97 \text{ \AA}$ and $\text{N--H} = 0.90 \text{ \AA}$, and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C, N})$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

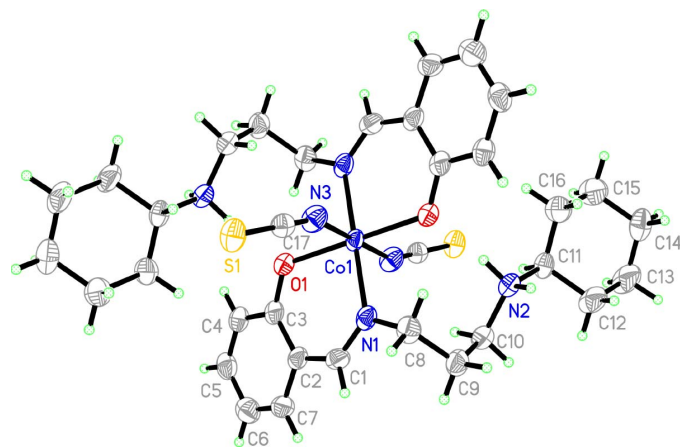


Figure 1

The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are generated by the symmetry operation $(-x, 1 - y, -z)$. H atoms are represented by small spheres.

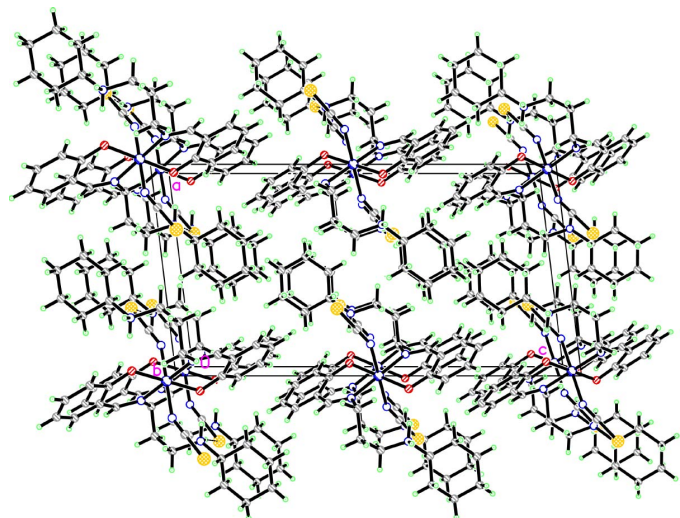


Figure 2

The crystal packing of (I), viewed along the b axis.

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