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cis-Bis[2-(cyclopropyliminomethyl)-6-methoxyphenolato]bis(thiocyanato)-cobalt(II)

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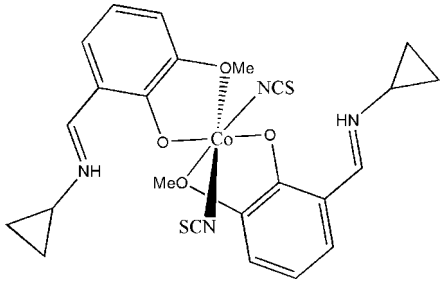
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.053; wR factor = 0.130; data-to-parameter ratio = 18.2.

In the title compound, $[Co(NCS)_2(C_{11}H_{13}NO_2)_2]$, a mononuclear Schiff base cobalt(II) complex, the Co atom is six-coordinated by four O atoms from two Schiff base ligands, and by two N atoms from two thiocyanate ligands, forming a distorted octahedral geometry. The central Co atom lies on a twofold rotation axis. An intramolecular N—H···O hydrogen bond is present.

Related literature

For related literature, see: Di Bella *et al.* (1997); Kraihanzel *et al.* (1981); Loeb *et al.* (1984); Mukhopadhyay *et al.* (2003); Wang (2007*a*,*b*).



Experimental

Crystal data

$[Co(NCS)_2(C_{11}H_{13}NO_2)_2]$
M_r = 557.54
Monoclinic, $C2/c$
a = 21.851 (3) Å
b = 7.6424 (11) Å
c = 16.073 (2) Å
β = 103.196 (3)°
V = 2613.2 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.85 mm^{-1}
T = 298 (2) K
0.23 × 0.20 × 0.17 mm

Data collection

Bruker SMART APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.828, T_{max} = 0.869
10900 measured reflections
2962 independent reflections
1960 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.130
S = 1.05
2962 reflections
163 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	1.997 (2)	Co1—O2	2.387 (2)
Co1—N2	2.031 (3)		
O1^i—Co1—O1	148.34 (13)	O1^i—Co1—O2	86.55 (8)
O1^i—Co1—N2	106.91 (9)	O1—Co1—O2	71.97 (8)
O1—Co1—N2	92.76 (9)	N2^i—Co1—O2	82.96 (10)
N2^i—Co1—N2	103.17 (16)	N2—Co1—O2	164.69 (9)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.901 (10)	1.93 (3)	2.609 (3)	131 (3)

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GD2028).

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supplementary materials

Acta Cryst. (2008). E**64**, m78 [**doi:10.1107/S1600536807062186**]

cis-Bis[2-(cyclopropyliminomethyl)-6-methoxyphenolato]bis(thiocyanato)cobalt(II)

S.-X. Wang

Comment

Schiff base complexes have been studied extensively due to their interesting structures and numerous applications (Mukhopadhyay *et al.*, 2003; Kraihanzel *et al.*, 1981; Di Bella *et al.*, 1997; Loeb *et al.*, 1984). Previously, the author has reported the crystal structure of a Schiff base zinc(II) complex (Wang, 2007*a*) and a Schiff base nickel(II) complex (Wang, 2007*b*). As part of a further investigation of Schiff base complexes, the structure of the title compound, a mononuclear cobalt(II) complex, is reported here.

The octahedral coordination environment of Co^{II} atom in the title compound is formed by four O atoms from two Schiff base ligands, and by two N atoms from two thiocyanate ligands (Fig. 1). The central Co atom lies on a twofold axis symmetry position·The coordination bond distances and angles are listed in Table 1.

Experimental

The title compound was obtained by stirring of 3-methoxysalicylaldehyde (0.2 mmol, 30.5 mg), cyclopropylamine (0.2 mmol, 11.5 mg), ammonium thiocyanate (0.2 mmol, 15.2 mg), and cobalt(II) acetate (0.1 mmol, 25.0 mg) in methanol (20 ml) for 30 min. The reaction mixture was then filtered. Brown block-shaped single crystals suitable for X-ray diffraction were formed from the filtrate after nine days.

Refinement

H1 was located from a difference Fourier map and refined isotropically, with N—H distance restrained to 0.90 (1) Å. Other H atoms were positioned geometrically (C—H = 0.93–0.98 Å) and refined as riding, with U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

Figures

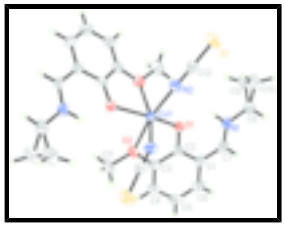

Fig. 1. The molecular structure of title compound, showing the numbering scheme and displacement ellipsoids drawn at the 30% probability level

cis-Bis[2-(cyclopropyliminomethyl)-6-methoxyphenolato]bis(thiocyanato)cobalt(II)

Crystal data

$[Co(NCS)_2(C_{11}H_{13}NO_2)_2]$ F_{000} = 1156

M_r = 557.54	D_x = 1.417 Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 1290 reflections
a = 21.851 (3) Å	θ = 2.5–24.3º
b = 7.6424 (11) Å	μ = 0.85 mm^{-1}
c = 16.073 (2) Å	T = 298 (2) K
β = 103.196 (3)º	Block, brown
V = 2613.2 (6) Å^3	0.23 × 0.20 × 0.17 mm
Z = 4	

Data collection

Bruker SMART APEX area-detector diffractometer	2962 independent reflections
Radiation source: fine-focus sealed tube	1960 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.055
T = 298(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −27→28
T_{min} = 0.828, T_{max} = 0.869	k = −9→9
10900 measured reflections	l = −20→20

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.053	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.130	$w = 1/[\sigma^2(F_o^2) + (0.0516P)^2 + 0.3065P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$
2962 reflections	$\Delta\rho_{max}$ = 0.39 e Å^{-3}
163 parameters	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.5000	0.87110 (8)	0.2500	0.0439 (2)
N1	0.41206 (13)	0.8517 (4)	−0.02768 (16)	0.0525 (7)
N2	0.42546 (13)	1.0362 (4)	0.23494 (17)	0.0583 (7)
O1	0.47825 (9)	0.7998 (3)	0.12725 (12)	0.0507 (5)
O2	0.57533 (10)	0.6595 (3)	0.22880 (14)	0.0590 (6)
S1	0.30172 (5)	1.14011 (15)	0.17478 (7)	0.0854 (4)
C1	0.51623 (15)	0.7354 (4)	0.00295 (19)	0.0491 (8)
C2	0.52171 (13)	0.7346 (4)	0.09220 (18)	0.0437 (7)
C3	0.57669 (14)	0.6617 (4)	0.1437 (2)	0.0485 (8)
C4	0.62403 (15)	0.6003 (4)	0.1085 (2)	0.0621 (9)
H4	0.6601	0.5533	0.1435	0.075*
C5	0.61837 (18)	0.6079 (5)	0.0207 (3)	0.0704 (11)
H5	0.6511	0.5680	−0.0025	0.085*
C6	0.56587 (17)	0.6727 (4)	−0.0313 (2)	0.0626 (9)
H6	0.5625	0.6760	−0.0900	0.075*
C7	0.46021 (15)	0.7952 (4)	−0.0526 (2)	0.0529 (8)
H7	0.4582	0.7934	−0.1110	0.063*
C8	0.35288 (18)	0.8950 (6)	−0.0835 (2)	0.0759 (11)
H8	0.3544	0.9178	−0.1429	0.091*
C9	0.29577 (17)	0.8083 (6)	−0.0720 (3)	0.0946 (14)
H9A	0.2646	0.7756	−0.1228	0.114*
H9B	0.2995	0.7282	−0.0242	0.114*
C10	0.30497 (19)	0.9911 (6)	−0.0532 (3)	0.0912 (13)
H10A	0.3144	1.0262	0.0064	0.109*
H10B	0.2795	1.0735	−0.0922	0.109*
C11	0.63187 (18)	0.6133 (5)	0.2889 (3)	0.0874 (13)
H11A	0.6403	0.4911	0.2835	0.131*
H11B	0.6271	0.6368	0.3458	0.131*
H11C	0.6662	0.6810	0.2779	0.131*
C12	0.37396 (16)	1.0796 (4)	0.2087 (2)	0.0510 (8)
H1	0.4126 (16)	0.857 (4)	0.0285 (8)	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0370 (3)	0.0611 (4)	0.0314 (3)	0.000	0.0029 (2)	0.000
N1	0.0502 (16)	0.0656 (18)	0.0380 (14)	−0.0084 (13)	0.0025 (13)	0.0051 (13)
N2	0.0484 (16)	0.0724 (19)	0.0538 (16)	0.0111 (14)	0.0109 (13)	−0.0032 (14)
O1	0.0378 (11)	0.0764 (14)	0.0359 (11)	0.0060 (10)	0.0045 (9)	−0.0060 (10)

O2	0.0489 (13)	0.0754 (16)	0.0477 (13)	0.0137 (11)	0.0003 (10)	0.0001 (11)
S1	0.0532 (6)	0.0992 (8)	0.0930 (8)	0.0165 (5)	−0.0054 (5)	0.0037 (6)
C1	0.0559 (19)	0.0499 (19)	0.0434 (18)	−0.0123 (15)	0.0151 (15)	−0.0048 (14)
C2	0.0393 (16)	0.0477 (18)	0.0439 (17)	−0.0078 (13)	0.0094 (13)	−0.0066 (14)
C3	0.0420 (18)	0.0489 (18)	0.0534 (19)	−0.0044 (13)	0.0085 (15)	−0.0040 (14)
C4	0.0458 (19)	0.062 (2)	0.079 (3)	0.0045 (16)	0.0149 (18)	−0.0026 (18)
C5	0.061 (2)	0.075 (3)	0.087 (3)	−0.0018 (19)	0.040 (2)	−0.012 (2)
C6	0.069 (2)	0.071 (2)	0.056 (2)	−0.0079 (19)	0.0313 (19)	−0.0101 (17)
C7	0.062 (2)	0.062 (2)	0.0357 (17)	−0.0158 (17)	0.0126 (16)	−0.0028 (15)
C8	0.059 (2)	0.118 (3)	0.0442 (19)	−0.004 (2)	0.0002 (17)	0.012 (2)
C9	0.051 (2)	0.090 (3)	0.131 (4)	−0.004 (2)	−0.006 (2)	0.001 (3)
C10	0.076 (3)	0.081 (3)	0.104 (3)	0.019 (2)	−0.006 (2)	0.010 (3)
C11	0.069 (3)	0.112 (3)	0.069 (3)	0.035 (2)	−0.009 (2)	0.014 (2)
C12	0.059 (2)	0.0513 (19)	0.0439 (18)	0.0003 (16)	0.0133 (15)	−0.0017 (15)

Geometric parameters (Å, °)

Co1—O1^{i}	1.997 (2)	C3—C4	1.371 (4)
Co1—O1	1.997 (2)	C4—C5	1.389 (5)
Co1—N2^{i}	2.031 (3)	C4—H4	0.9300
Co1—N2	2.031 (3)	C5—C6	1.350 (5)
Co1—O2	2.387 (2)	C5—H5	0.9300
Co1—O2^{i}	2.387 (2)	C6—H6	0.9300
N1—C7	1.283 (4)	C7—H7	0.9300
N1—C8	1.434 (4)	C8—C10	1.451 (5)
N1—H1	0.901 (10)	C8—C9	1.461 (5)
N2—C12	1.157 (4)	C8—H8	0.9800
O1—C2	1.308 (3)	C9—C10	1.434 (6)
O2—C3	1.375 (4)	C9—H9A	0.9700
O2—C11	1.428 (4)	C9—H9B	0.9700
S1—C12	1.615 (4)	C10—H10A	0.9700
C1—C6	1.408 (4)	C10—H10B	0.9700
C1—C2	1.412 (4)	C11—H11A	0.9600
C1—C7	1.416 (4)	C11—H11B	0.9600
C2—C3	1.409 (4)	C11—H11C	0.9600
O1^{i}—Co1—O1	148.34 (13)	C6—C5—C4	120.7 (3)
O1^{i}—Co1—N2^{i}	92.76 (9)	C6—C5—H5	119.6
O1—Co1—N2^{i}	106.91 (9)	C4—C5—H5	119.6
O1^{i}—Co1—N2	106.91 (9)	C5—C6—C1	120.3 (3)
O1—Co1—N2	92.76 (9)	C5—C6—H6	119.9
N2^{i}—Co1—N2	103.17 (16)	C1—C6—H6	119.9
O1^{i}—Co1—O2	86.55 (8)	N1—C7—C1	124.3 (3)
O1—Co1—O2	71.97 (8)	N1—C7—H7	117.8
N2^{i}—Co1—O2	82.96 (10)	C1—C7—H7	117.8
N2—Co1—O2	164.69 (9)	N1—C8—C10	121.6 (3)
O1^{i}—Co1—O2^{i}	71.97 (8)	N1—C8—C9	119.4 (3)

O1—Co1—O2^{i}	86.55 (8)	C10—C8—C9	59.0 (3)
N2^{i}—Co1—O2^{i}	164.69 (9)	N1—C8—H8	115.1
N2—Co1—O2^{i}	82.96 (10)	C10—C8—H8	115.1
O2—Co1—O2^{i}	94.69 (11)	C9—C8—H8	115.1
C7—N1—C8	124.7 (3)	C10—C9—C8	60.1 (3)
C7—N1—H1	120 (2)	C10—C9—H9A	117.8
C8—N1—H1	115 (2)	C8—C9—H9A	117.8
C12—N2—Co1	155.4 (3)	C10—C9—H9B	117.8
C2—O1—Co1	119.80 (17)	C8—C9—H9B	117.8
C3—O2—C11	117.7 (3)	H9A—C9—H9B	114.9
C3—O2—Co1	107.81 (17)	C9—C10—C8	60.9 (3)
C11—O2—Co1	126.1 (2)	C9—C10—H10A	117.7
C6—C1—C2	120.1 (3)	C8—C10—H10A	117.7
C6—C1—C7	119.7 (3)	C9—C10—H10B	117.7
C2—C1—C7	120.2 (3)	C8—C10—H10B	117.7
O1—C2—C3	120.2 (3)	H10A—C10—H10B	114.8
O1—C2—C1	122.3 (3)	O2—C11—H11A	109.5
C3—C2—C1	117.5 (3)	O2—C11—H11B	109.5
C4—C3—O2	126.6 (3)	H11A—C11—H11B	109.5
C4—C3—C2	121.0 (3)	O2—C11—H11C	109.5
O2—C3—C2	112.3 (3)	H11A—C11—H11C	109.5
C3—C4—C5	120.3 (3)	H11B—C11—H11C	109.5
C3—C4—H4	119.8	N2—C12—S1	178.3 (3)
C5—C4—H4	119.8		

Symmetry codes: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.901 (10)	1.93 (3)	2.609 (3)	131 (3)

Fig. 1