Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Aqua(isothiocyanato){2,2′-[propane-1,3-diylbis(nitrilomethylidyne)]diphenolato}cobalt(III)

Yu-Xi Sun

Department of Chemistry, Qufu Normal University, Qufu 273165, People's Republic of China

Correspondence e-mail: yuxisun@163.com

Received 24 November 2004
Accepted 29 November 2004
Online 4 December 2004

Key indicators

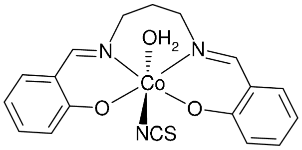
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.007 Å
R factor = 0.058
wR factor = 0.161
Data-to-parameter ratio = 15.6

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

The title compound, [Co($C_{17}H_{16}N_2O_2$)(NCS)(H_2O)], is a mononuclear cobalt(III) complex whose Co atom is coordinated by two N atoms and two O atoms of the Schiff base ligand, the N atom of the isothiocyanate anion, and a water molecule in a distorted octahedral configuration. The molecules are linked by intermolecular O—H···O hydrogen bonds to form chains parallel to *b*.

Comment

Complex (I) is a mononuclear cobalt(III) compound (Fig. 1). The Co^{III} atom is coordinated by two N atoms and two O atoms of the Schiff base dianion, the N atom of an isothiocyanate anion and a water molecule in a distorted octahedral configuration. The Schiff base ligand acts as a tetradentate ligand. The *trans* angles are close to 180°. The bond lengths of the Schiff base ligand are within normal ranges (Allen *et al.*, 1987). The six-membered chelate ring containing the Co atom, the azomethine N atoms and the three C atoms of the connecting 1,3-diaminopropane unit has a boat conformation.



(I)

In the crystal structure, the molecules are linked together by intermolecular O—H···O hydrogen bonds, forming chains parallel to the *b* axis (Table 1 and Fig. 2).

Experimental

Salicylaldehyde (0.2 mmol, 24.4 mg) and 1,3-diaminopropane (0.1 mmol, 7.4 mg) were dissolved in ethanol (10 ml). The mixture

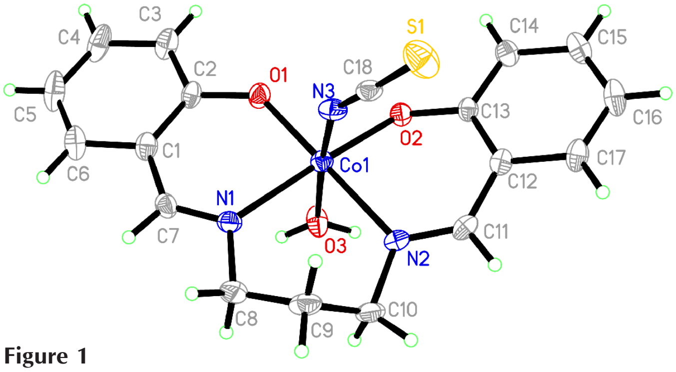


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

was stirred for 10 min to give a clear yellow solution. To the solution was added an ethanol solution (5 ml) of ammonium thiocyanate (0.1 mmol, 7.6 mg) and an aqueous solution (5 ml) of $Co(CH_3COO)_2 \cdot 4H_2O$ (0.1 mmol, 25.8 mg) with stirring. After allowing the brown filtrate to stand in air for 10 d, brown block-shaped crystals were isolated.

Crystal data

$[Co(C_{17}H_{16}N_2O_2)(NCS)(H_2O)]$
$M_r = 415.34$
Monoclinic, $P2_1/n$
$a = 12.7882\ (10)$ Å
$b = 6.9977\ (5)$ Å
$c = 21.3137\ (17)$ Å
$\beta = 105.994\ (1)°$
$V = 1833.5\ (2)$ Å^3
$Z = 4$
$D_x = 1.505$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 2671 reflections
$\theta = 3.0$–$24.7°$
$\mu = 1.07$ mm^{-1}
$T = 295\ (2)$ K
Block, brown
0.27 × 0.24 × 0.18 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.761$, $T_{max} = 0.830$
10267 measured reflections
3784 independent reflections
2944 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 26.5°$
$h = -11 \rightarrow 16$
$k = -8 \rightarrow 8$
$l = -26 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.161$
$S = 1.07$
3784 reflections
243 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.085P)^2 + 1.0593P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.98$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···O1^{i}	0.895 (10)	1.95 (2)	2.739 (4)	146 (3)
O3—H3*B*···O2^{i}	0.891 (10)	1.91 (3)	2.669 (4)	142 (3)

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

The H atoms of the water molecule were located in a difference Fourier map and refined isotropically, with the O—H and H···H distances restrained to 0.90 (1) and 1.47 (2) Å, respectively. The other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

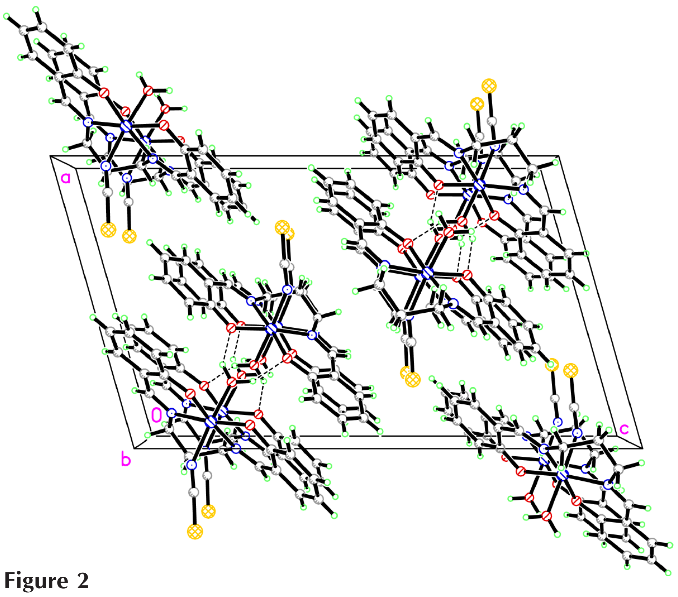


Figure 2
The crystal packing of (I), viewed along the *b* axis. Dashed lines show intermolecular hydrogen bonds.

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

The author thanks Qufu Normal University for a research grant.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans.* 2, pp. S1–19.
Bruker (2002). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS, Inc., Madison, Wisconsin, USA.