Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Aqua(1,10-phenanthroline)(thiodiglycolato)cobalt(II)

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.038
wR factor = 0.091
Data-to-parameter ratio = 15.9

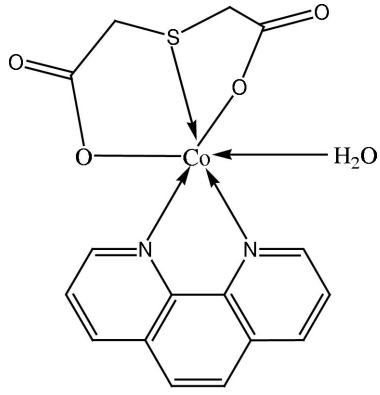
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 9 February 2005
Accepted 15 February 2005
Online 19 February 2005

In the title cobalt compound, $[Co(C_4H_4O_4S)(C_{12}H_8N_2)(H_2O)]$, the distorted octahedron around the Co atom is formed by the O atom from a water molecule, two N atoms from the heterocycle, two carboxyl O atoms and an S atom from the dianion. Hydrogen bonds extend the structure into a two-dimensional network.

Comment

The S atom of thiodiglycolic acid may be coordinated to metal atoms. However, only a few metal–thiodiglycolate complexes have been reported (Bonomo *et al.*, 1982; Baggio *et al.*, 1996, 1999; Kopel *et al.*, 2003; Grirrane *et al.*, 2003).



(I)

In the title compound, (I), the coordination polyhedron around the Co atom can be described as a distorted octahedron consisting of two N-atom donors from a 1,10-phenanthroline, one O atom from the water molecule and three donors from the thiodiglycolate ligand (Fig. 1 and Table 1). The flexible dicarboxylate dianion is converted to a rigid ligand when the S-atom donor coordinates to the Co^{II} atom, giving rise to the formation of two five-membered chelate rings. Both rings display a twist conformation. Each carboxyl group is coordinated in monodentate fashion to the cobalt centre. Both uncoordinated carboxyl O atoms form hydrogen bonds with water molecules, resulting in a two-dimensional hydrogen-bonding network (Fig. 2 and Table 2).

Experimental

A mixture of cobalt(II) acetate tetrahydrate (0.0747 g, 0.30 mmol), thiodiglycolic acid (0.0452 g, 0.30 mmol), 1,10-phenanthroline (0.0595 g, 0.30 mmol) and water (10 ml) was heated at 393 K for 24 h in a 20 ml Teflon-lined stainless steel autoclave. After cooling, blue block-shaped crystals of (I) were obtained.

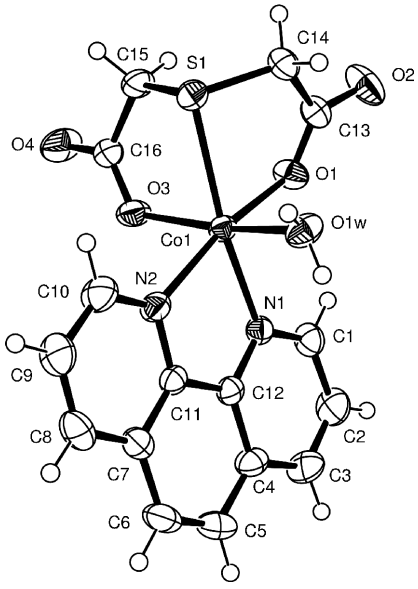


Figure 1
ORTEP-3 view (Farrugia, 1997) of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

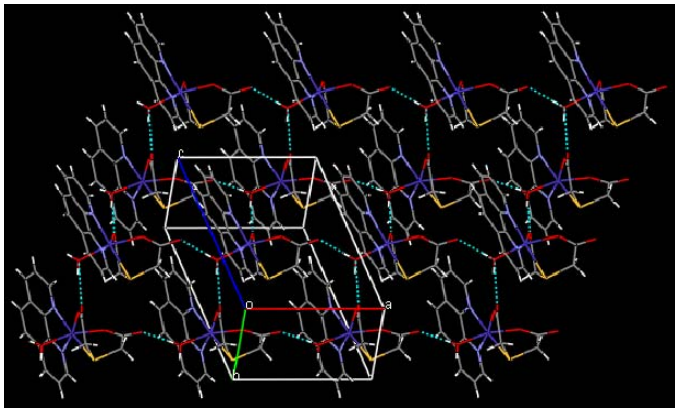


Figure 2
View of the two-dimensional hydrogen-bonding network of (I), with hydrogen bonds shown as dashed lines.

Crystal data

$[Co(C_4H_4O_4S)(C_{12}H_8N_2)(H_2O)]$	D_x = 1.670 Mg m^{-3}
M_r = 405.28	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 3581 reflections
a = 8.0127 (9) Å	θ = 2.8–24.7°
b = 22.524 (3) Å	μ = 1.23 mm^{-1}
c = 9.733 (1) Å	T = 295 (2) K
β = 113.420 (1)°	Block, blue
V = 1611.9 (3) Å^3	0.14 × 0.14 × 0.09 mm
Z = 4	

Data collection

Bruker SMART APEX area-detector diffractometer	3688 independent reflections
φ and ω scans	2997 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	R_{int} = 0.050
T_{min} = 0.784, T_{max} = 0.898	θ_{max} = 27.5°
18 142 measured reflections	$h = -10 \rightarrow 10$
	$k = -29 \rightarrow 29$
	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0432P)^2 + 0.4148P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.038	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.091	$\Delta\rho_{max}$ = 0.38 e Å^{-3}
S = 1.02	$\Delta\rho_{min}$ = −0.27 e Å^{-3}
3688 reflections	
232 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.033 (2)	Co1—N1	2.114 (2)
Co1—O3	2.038 (2)	Co1—N2	2.149 (2)
Co1—O1*W*	2.084 (2)	Co1—S1	2.5191 (7)
O1—Co1—O3	94.78 (8)	O1*W*—Co1—N2	88.34 (8)
O1—Co1—O1*W*	92.07 (8)	N1—Co1—N2	77.91 (7)
O3—Co1—O1*W*	166.26 (8)	O1—Co1—S1	80.51 (5)
O1—Co1—N1	91.64 (7)	O3—Co1—S1	81.51 (5)
O3—Co1—N1	100.60 (7)	O1*W*—Co1—S1	87.90 (5)
O1*W*—Co1—N1	91.08 (7)	N1—Co1—S1	172.03 (5)
O1—Co1—N2	169.55 (7)	N2—Co1—S1	109.95 (5)
O3—Co1—N2	87.07 (7)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O2^{i}	0.84 (1)	1.93 (1)	2.764 (3)	170 (3)
O1*W*—H1*W*2···O4^{ii}	0.85 (3)	1.82 (3)	2.662 (3)	179 (3)

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

The H atoms bonded to C atoms were positioned geometrically and included in the refinement using the riding-model approximation [C—H = 0.93 Å for CH and C—H = 0.97 Å for CH_2, and U_{iso}(H) = 1.2U_{eq}(C)]. The water H atoms were located in a difference Fourier map and refined with distance restraints of O—H = 0.85 (1) Å and with fixed isotropic displacement parameters of U_{iso}(H) = 0.05 Å^2.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

We thank Professor Seik Weng Ng for his kind help in the single-crystal structure analysis and reference information and the National Natural Science Foundation of China (grant No. 50073019).

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