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Aqua(2,2′-diamino-4,4-bi-1,3-thiazole-κ²N,N′)(oxydiacetato-κ³O,O′,O″)cobalt(II) monohydrate

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In the title complex, $[Co(C_4H_4O_5)(C_6H_6N_4S_2)(H_2O)]\cdot H_2O$, the Co^{II} atom has a distorted octahedral coordination geometry, formed by one tridentate oxydiacetate, one bidentate diaminobithiazole and one coordinated water molecule. The Co^{II} atom lies on a crystallographic twofold axis, resulting in disorder of the oxydiacetate dianion and the coordinated water. In the crystal structure, parallel thiazole rings are separated by 3.343 (4) Å, allowing π–π stacking interactions to occur.

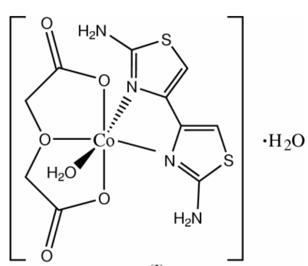
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.022
wR factor = 0.060
Data-to-parameter ratio = 10.1

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

Comment

Metal complexes with 2,2′-diamino-4,4′-bithiazole (DABT) or its derivatives show potential application in some fields. For example, Co^{II} and Ni^{II} complexes with DABT have been found to be effective inhibitors of DNA synthesis in tumor cells (Waring, 1981; Fisher *et al.*, 1985), while multinuclear Fe^{II} and Cu^{II} complexes with DABT Schiff base have been found to be potential soft magnetic materials (Sun *et al.*, 1997). As part of a structural investigation of these complexes, we present here the X-ray structure of the title cobalt(II) complex with DABT, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The Co^{II} atom lies on a crystallographic twofold axis, resulting in disorder of the oxydiacetate dianion and the coordinated water molecule. The Co^{II} atom has a distorted octahedral coordination geometry (Table 1), formed by one DABT, one oxydiacetate dianion (ODA) and one coordinated water molecule. The tridentate ODA ligand chelates to the Co atom in a meridional configuration, with an O1—Co—O4 bond angle of 147.73 (9)°. A water molecule coordinates the Co atom, with a Co—O bond of 2.274 (18) Å. The DABT chelates to the Co atom, showing a planar configuration; the maximum atomic deviation is 0.0535 (18) Å for atom C5. This differs from the twisted thiazole rings found in the Cd^{II} complex dichlorobis(DABT)cadmium(II) (Liu *et al.*, 2003). The amino groups of DABT form intramolecular hydrogen bonds with the coordinated water and ODA ligand, thus stabilizing the molecular structure. An uncoordinated water molecule links

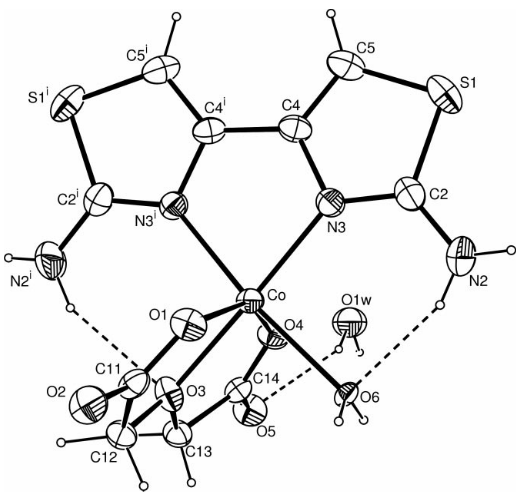


Figure 1
The structure of (I), shown with 40% probability displacement ellipsoids. Only one of the two disordered components of the oxydiacetate ligand and the coordinated water molecule are shown. Dashed lines indicate the hydrogen bonding. [Symmetry code: (i) $1 - x, y, \frac{1}{2} - z$.]

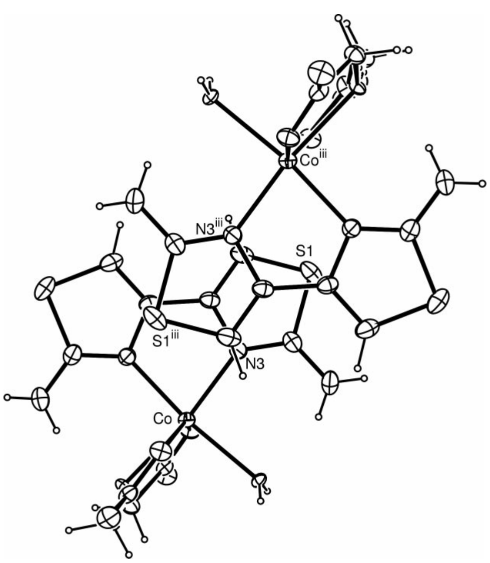


Figure 2
The π–π stacking of thiazole rings in neighboring complex molecules. [Symmetry code: (iii) $1 - x, -y, -z$.]

to the complex *via* an O—H···O hydrogen bond (Table 2).

In the crystal structure, parallel thiazole rings are separated by 3.343 (4) Å, allowing the existence of π–π stacking interactions (Fig. 2).

Experimental

Fine crystals of DABT were obtained according to the method of Erlenmeyer (1948). An aqueous solution (10 ml) of DABT (0.10 g, 0.5 mmol) and $CoCl_2 \cdot 6H_2O$ (0.12 g, 0.5 mmol) was mixed with an aqueous solution of ODA (0.07 g, 0.5 mmol) and NaOH (0.04 g 1 mmol), and refluxed for 3 h. The salmon-pink solution was cooled to room temperature and filtered. Single crystals of the title compound were obtained from the filtrate after 2 d.

Crystal data

$[Co(C_4H_4O_5)(C_6H_6N_4S_2)(H_2O)] \cdot H_2O$
$M_r = 425.32$
Monoclinic, $C2/c$
$a = 8.1393$ (16) Å
$b = 22.855$ (2) Å
$c = 8.6530$ (19) Å
$\beta = 100.633$ (16)°
$V = 1582.1$ (5) Å^3
$Z = 4$
$D_x = 1.786$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 20 reflections
$\theta = 9.5$–$12.2°$
$\mu = 1.39$ mm^{-1}
$T = 295$ (2) K
Prism, red
$0.52 \times 0.48 \times 0.30$ mm

Data collection

Rigaku AFC-7*S* diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.48$, $T_{max} = 0.66$
1669 measured reflections
1558 independent reflections
1414 reflections with $I > 2\sigma(I)$
$R_{int} = 0.011$
$\theta_{max} = 26.0°$
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 28$
$l = -10 \rightarrow 10$
3 standard reflections every 150 reflections intensity decay: 0.2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.022$
$wR(F^2) = 0.060$
$S = 1.06$
1558 reflections
155 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0288P)^2 + 1.5071P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co—O1	2.057 (5)	Co—O3	2.105 (19)
Co—O4	2.068 (5)	Co—O6	2.274 (18)
Co—N3	2.0946 (15)		
O1—Co—O4	147.73 (9)	N3—Co—O3	175.0 (5)
O1—Co—N3	109.87 (13)	O1—Co—O6	86.4 (4)
O4—Co—N3	102.05 (12)	O4—Co—O6	87.3 (4)
O1—Co—O3	74.3 (5)	N3—Co—O6	92.9 (5)
O4—Co—O3	74.1 (5)	O3—Co—O6	90.09 (15)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1···O5	0.88	2.11	2.835 (3)	140
O1*W*—H1···O2^{i}	0.88	2.10	2.852 (3)	144
N2—H2*A*···O6	0.87	2.09	2.903 (14)	155
N2—H2*A*···O3^{i}	0.87	2.28	3.067 (16)	151
N2—H2*B*···O1*W*^{ii}	0.84	2.41	3.174 (3)	151

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

The thiazole H atom was placed in a calculated position, with C—H = 0.93 Å, and included in the final cycles of refinement in the riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms of the coordinated water molecule were placed in theoretical positions (Nardelli, 1999), while other H atoms were located in a difference Fourier map. These H atoms were included in structure-factor calculations with fixed positional parameters and isotropic displacement parameters of 0.05 Å^2.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1985); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); *WinGX* (Farrugia, 1999).

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