metal-organic papers

(2,2'-Diamino-4,4'-bi-1,3-thiazole-κ^2N,N')-bis(glycinato-κ^2N,O)cobalt(II) dihydrate

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In the title compound, [Co(C₂H₄NO₂)₂(C₆H₆N₂S)]·2H₂O, the Co^{II} ion (site symmetry 2) is coordinated by an N,N-bidentate diaminobithiazole ligand and two N,O-bidentate glycinate anions in a distorted octahedral geometry. The five-membered Co–glycinate ring displays an envelope conformation. A network of O—H···O and N—H···O hydrogen bonds helps to consolidate the crystal packing.

Comment

Complexes containing the diaminobithiazole (DABT) ligand have attracted much attention because of their interesting magnetic properties (Sun et al., 1997). As part of an ongoing investigation of metal complexes incorporating DABT (Liu *et al.*, 2001), the title Co^{II} complex, (I), has been prepared and its crystal structure is presented here. The asymmetric unit consist of a Co^{II} ion (site symmetry 2), half a DABT molecule, a glycinate anion and a water molecule.

(I)
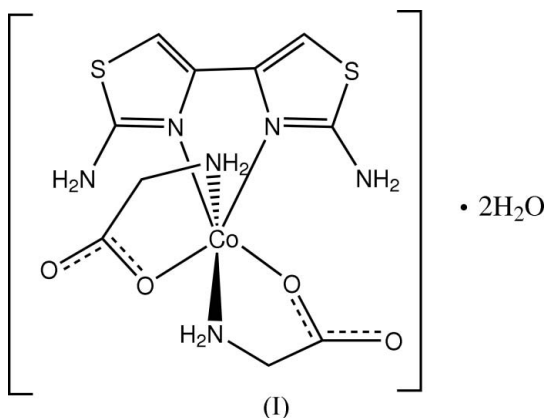
Crystal symmetry results in the Co^{II} ion being coordinated by two glycinate anions and one DABT molecule, with a distorted *cis*-CoN_4O_2 octahedral geometry (Fig. 1 and Table 1). The DABT molecule chelating to the Co^{II} ion is close to being planar; the dihedral angle of 9.68 (6)° in (I) between the thiazole mean planes is comparable to the values of 11.1 (4)° in an Ni^{II} complex of DABT (Liu & Xu, 2004) and 10.3 (3)° in another Co^{II} complex of DABT (Liu *et al.*, 2003).

The glycinate anion chelates to the Co^{II} ion through the amino N atom and a carboxyl O atom. The chelate five-membered ring displays an envelope conformation, with atom N3 lying at the flap position and displaced from the mean plane formed by the other four atoms by 0.399 (2) Å. The uncoordinated carboxyl O2 atom links to two neighbouring complex molecules and one non-coordinated water molecule *via* N—H···O and O—H···O hydrogen bonds (Table 2).

Experimental

An aqueous solution (20 ml) containing DABT (0.20 g, 1 mmol) and $CoCl_2\cdot6H_2O$ (0.24 g, 1 mmol) was mixed with another aqueous solution (10 ml) of glycine (0.15 g, 2 mmol) and NaOH (0.04 g, 1 mmol). The mixture was refluxed for 5 h. The solution was filtered after cooling to room temperature. Red single crystals of (I) were obtained from the filtrate after 3 d.

Crystal data

$[Co(C_2H_4NO_2)_2(C_6H_6N_2S)]\cdot2H_2O$	$D_x = 1.765$ Mg m^{-3}
$M_r = 441.35$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 8864
$a = 13.1155$ (12) Å	reflections
$b = 8.9953$ (11) Å	$\theta = 2.9–25.2°$
$c = 14.0924$ (12) Å	$\mu = 1.33$ mm^{-1}
$\beta = 92.590$ (2)°	$T = 294$ (2) K
$V = 1660.9$ (3) Å^3	Prism, red
$Z = 4$	$0.30 \times 0.22 \times 0.15$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer	2063 independent reflections
ω scans	1924 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$R_{int} = 0.024$
$T_{min} = 0.720$, $T_{max} = 0.820$	$\theta_{max} = 28.3°$
9452 measured reflections	$h = -16 \rightarrow 17$
	$k = -10 \rightarrow 11$
	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0376P)^2 + 1.092P]$
$R[F^2 > 2\sigma(F^2)] = 0.024$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.066$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.06$	$\Delta\rho_{max} = 0.34$ e Å^{-3}
2063 reflections	$\Delta\rho_{min} = -0.38$ e Å^{-3}
114 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Co—O1	2.1300 (10)	Co—N3	2.1367 (12)
Co—N1	2.1533 (11)		
C2—S—C1	89.61 (7)		

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1W—H1A$\cdots$O2^i	0.88	2.01	2.878 (2)	167
O1W—H1B$\cdots$O1^{ii}	0.88	2.19	2.965 (2)	146
N2—H2A$\cdots$O1^{ii}	0.85	2.39	3.097 (2)	142
N2—H2B$\cdots$O2^{iii}	0.87	2.09	2.915 (2)	158
N3—H3A$\cdots$O1W	0.89	2.25	3.073 (2)	154
N3—H3B$\cdots$O2^{iv}	0.87	2.45	3.297 (2)	163

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

H atoms bonded to C atoms were placed in calculated positions, with C—H = 0.93 (aromatic) or 0.97 Å (methylene) and included in
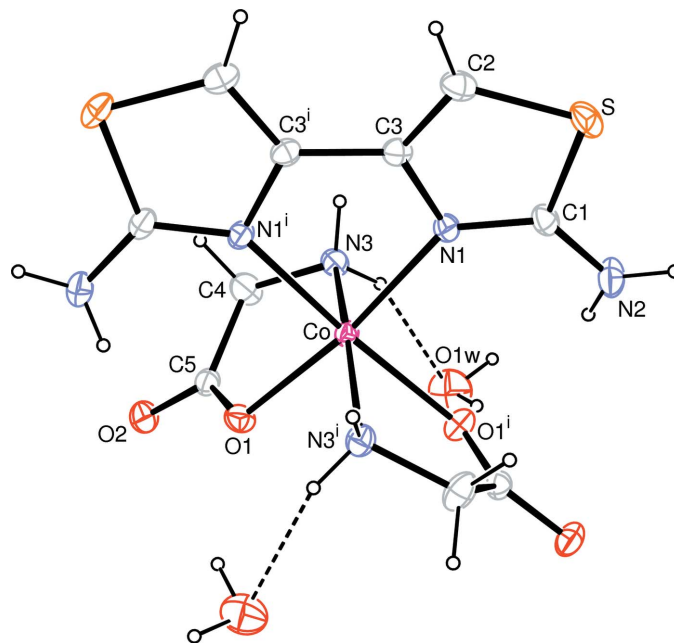
Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). Dashed lines indicate hydrogen bonds [symmetry code: (i) $-x + 1, y, -z + \frac{1}{2}$].

the final cycles of refinement in the riding mode, with $U_{iso}(H) = 1.2U_{eq}(C)$. Other H atoms were located in a difference Fourier map and refined as riding in their as-found relative positions, with $U_{iso}(H) = 1.5U_{eq}$(carrier).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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