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Diacetatobis(2-aminobenzothiazole-*κN*)cobalt(**II**)

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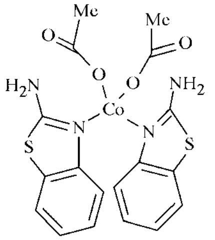
The title complex, $[Co(C_2H_3O_2)_2(C_7H_6N_2S)_2]$, contains a Co centre with a slightly distorted tetrahedral coordination geometry, involving two acetate ligands and two N atoms from the thiazole moiety [Co—O = 2.0025 (14) and 1.9953 (16) Å, and Co—N = 2.0524 (18) and 2.0568 (18) Å]. The interplanar angle between the two benzothiazole moieties is 77.86 (3)°. The amine groups, acting as donors, participate in intra- and intermolecular N—H···O hydrogen bonds, with N···O distances in the range 2.806 (2)–2.857 (2) Å.

Comment

Small and simple heterocyclic structures often exhibit complex biological properties. Substituted benzothiazoles show anti-tumour (Goldfarb *et al.*, 1999), anti-infective and antifungal (Sener *et al.*, 2000), and antihelmintic activities (Nadkarn *et al.*, 2000). Bis(benzothiazole) compounds have been studied as potential mimics for metalloproteins (Thompson *et al.*, 1982), and it is well known that N and S atoms play a key role in the coordination of metals at the active sites of numerous metallobiomolecules (Karlin & Zubieta, 1983). The structures of many metal complexes of 2-amino-1,3-thiazole derivatives, where the metal is directly bound to the ligand, are known, and these complexes include most of the first-row transition metals (*i.e.* Mn–Zn). In all but a few cases, the thiazole moieties bind to the metal *via* endocylic N atoms (Lynch & Duckhouse, 2001; Usman *et al.*, 2003). We report here the X-ray crystal structure of the title compound, (I).



(I)

In the molecular structure of (I) (Fig. 1), the two benzothiazole moieties form a dihedral angle of 77.86 (3)°. It is noteworthy that the two amine groups are not both located on the same side, because of steric hindrance. Both benzothiazole moieties are nearly planar, the largest deviation from the plane being that of atom C2 [0.026 (1) Å]. The cobalt centre, coordinated by two endocylic N atoms from the thiazole moieties and two acetate ligands (Co—N—C—N and

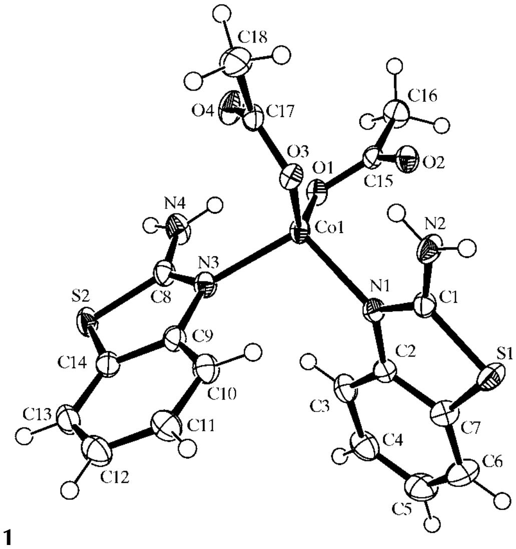


Figure 1
An *ORTEP-3* (Farrugia, 1997) drawing of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

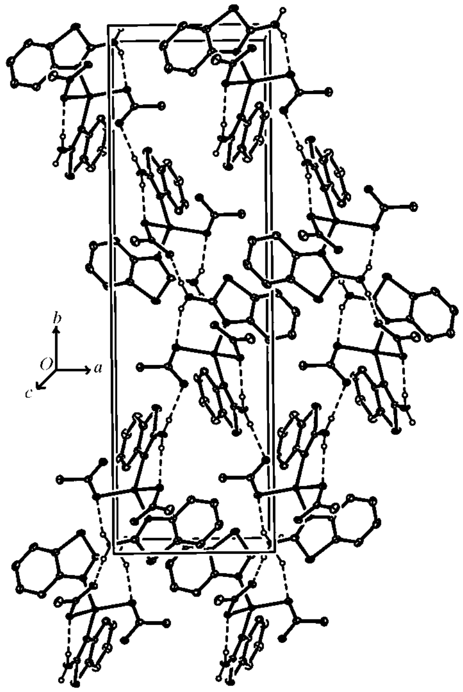


Figure 2
A view of the hydrogen-bonding interactions in (I). For clarity, H atoms bonded to C atoms have been omitted. Displacement ellipsoids are drawn at the 30% probability level and hydrogen bonds are shown as dashed lines.

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Co—O—C—C), adopts a synperiplanar and an antiperiplanar conformation, respectively. This CoN_2O_2 coordination forms a slightly distorted tetrahedral geometry, the angles around the Co atom ranging from 100.22 (7) to 128.90 (7)°. The bond lengths and angles in (I) are shown in Table 1. The C1—N1, C1—N2, C8—N3 and C8—N4 bonds are somewhat shorter than the C2—N1 and C9—N3 bonds, as a result of pronounced delocalization in the –N—C═N– fragment of the 2-aminobenzothiazole ring. The amine groups of both thiazole ligands are hydrogen bonded to the O atoms of the acetate ligands by intra- and intermolecular hydrogen bonds (Table 2). The $N2—H2B\cdots O2^{i}$ hydrogen bonds interconnect the molecules into chains along the *a* direction, and these are further interconnected into a three-dimensional network by $N4—H4B\cdots O4^{ii}$ hydrogen bonds (Fig. 2; symmetry codes as in Table 2).

Experimental

An ethanol solution of 2-aminobenzothiazole (4 mmol in 10 ml of ethanol) was added dropwise to $Co(CH_3COO)_2\cdot 6H_2O$ (2 mmol in 5 ml of ethanol) with stirring. The colour of the solution changed immediately to violet. The mixture was refluxed for 2 h and the resulting solution was kept at room temperature. After several days, violet crystals were obtained and dried under vacuum.

Crystal data

$[Co(C_2H_3O_2)_2(C_7H_6N_2S)_2]$
$M_r = 477.43$
Orthorhombic, $Pna2_1$
$a = 8.3049\ (4)$ Å
$b = 27.1833\ (16)$ Å
$c = 8.9868\ (5)$ Å
$V = 2028.81\ (19)$ Å^3
$Z = 4$
$D_x = 1.563$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 22768 reflections
$\theta = 1.5$–26.2°
$\mu = 1.09$ mm^{-1}
$T = 100$ K
Prism, violet
0.29 × 0.18 × 0.11 mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min} = 0.613$, $T_{max} = 0.830$
23485 measured reflections
3861 independent reflections

3697 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 26.1°$
$h = -10 \rightarrow 10$
$k = -33 \rightarrow 33$
$l = -9 \rightarrow 11$

Table 1
Selected geometric parameters (Å, °).

Co1—O3	1.9953 (16)	O4—C17	1.244 (3)
Co1—O1	2.0025 (14)	N1—C1	1.320 (3)
Co1—N1	2.0524 (18)	N1—C2	1.391 (3)
Co1—N3	2.0568 (18)	N2—C1	1.324 (3)
O1—C15	1.280 (3)	N3—C8	1.325 (3)
O2—C15	1.250 (3)	N3—C9	1.408 (3)
O3—C17	1.283 (3)	N4—C8	1.325 (3)
Co1—N1—C1—N2	7.8 (3)	Co1—O1—C15—C16	−171.31 (17)
Co1—N3—C8—N4	1.9 (3)	Co1—O3—C17—C18	179.22 (16)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N2—H2$A\cdots$O3	0.86	2.03	2.806 (2)	150
N2—H2$B\cdots$O2^{i}	0.86	2.01	2.857 (2)	167
N4—H4$A\cdots$O1	0.86	2.07	2.850 (2)	150
N4—H4$B\cdots$O4^{ii}	0.86	2.00	2.811 (3)	156

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

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.063$
$S = 1.04$
3861 reflections
264 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.046P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.50$ e Å^{-3}
Absolute structure: Flack (1983), 1720 Friedel pairs
Flack parameter: −0.005 (10)

All H atoms were placed in calculated positions, with C—H distances of 0.93 and 0.96 Å, and N—H distances of 0.86 Å. The U_{iso}(H) values were constrained to be 1.2 (1.5 for methyl groups) times U_{eq} of the carrier atom.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990); 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).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FR1521). Services for accessing these data are described at the back of the journal.

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