

## Diacetatobis(2-aminobenzothiazole)zinc(II)

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## Key indicators

Single-crystal X-ray study

$T = 293\text{ K}$

Mean  $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$

$R$  factor = 0.024

$wR$  factor = 0.060

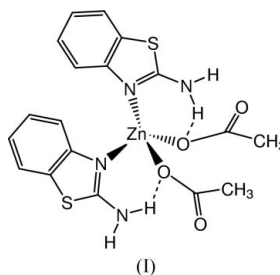
Data-to-parameter ratio = 14.4

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

In the title compound,  $[\text{Zn}(\text{C}_2\text{H}_3\text{O}_2)_2(\text{C}_7\text{H}_6\text{N}_2\text{S})_2]$ , the Zn atom is four-coordinated in the  $\text{ZnO}_2\text{N}_2$  form in a distorted tetrahedral geometry. The amino groups act as donors in  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds. Two intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds interconnect the molecules into a three-dimensional network. The planes of the acetate ligands are nearly orthogonal, and the Zn atom is displaced slightly from these two planes.

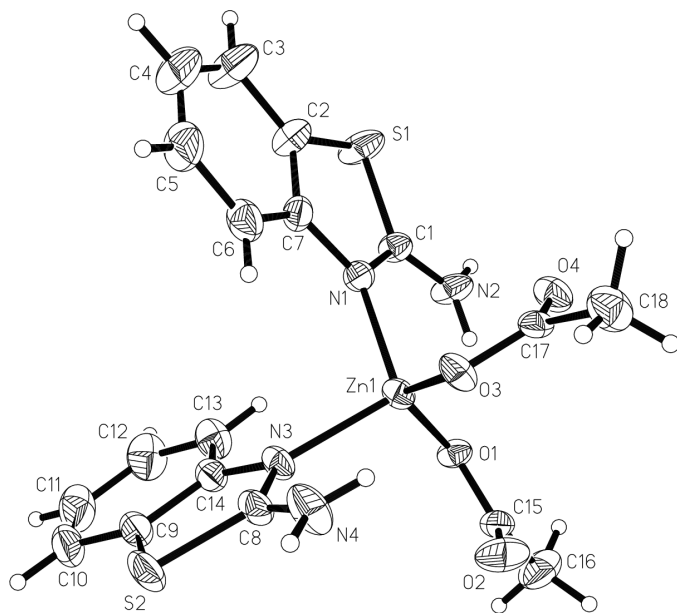
## Comment

The 1,3-thiazole derivatives constitute an important type of S,N-containing heterocycle (Raper, 1994; Metzger, 1984; Livingstone, 1987; House, 1987; Hantzsch & Winkler, 1987). The great interest in thiazoles and their derivatives is due to their biological importance as constituents of many biomolecules, including antibiotics. In some cases, the pharmacological activity of copper(II)-thiazole complexes was found to be much higher than that of the parent heterocycles (Chang *et al.*, 1982). However, the crystal structures of their complexes are unknown. An X-ray crystal structure analysis of the title compound, (I), was undertaken, and the results are reported here.



In (I), the  $\text{Zn}^{\text{II}}$  atom is four-coordinated by one N atom from each of two 2-aminobenzothiazole ligands and one O atom from each of two monodentate acetate anions. This  $\text{ZnO}_2\text{N}_2$  coordination forms a distorted tetrahedral geometry with a local non-crystallographic  $C_2$  symmetry and the range of angles around the Zn atom is  $102.3(1)$ – $125.1(1)^\circ$ . This type of coordination of Zn is also observed in the structures of zinc(II)-thiazole complexes reported previously (McCleverty *et al.*, 1980).

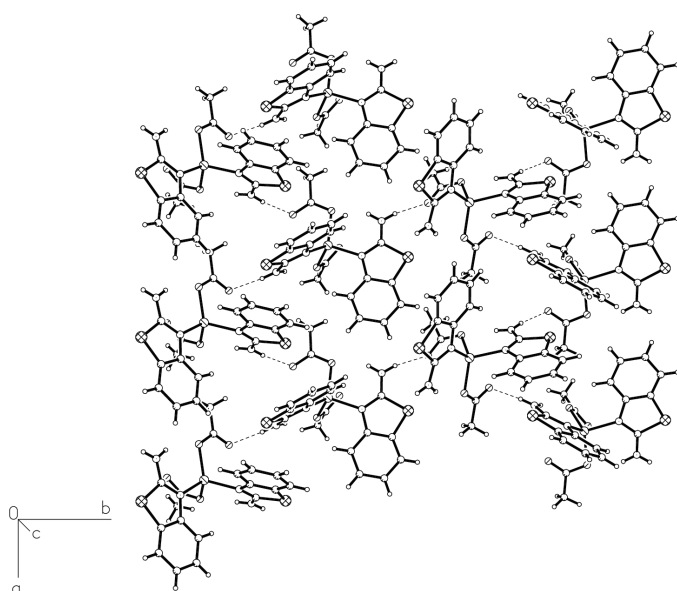
The two Zn–N bond lengths (Table 1) are similar, and agree with that in another zinc(II)-thiazole complex [ $2.061(2)\text{ \AA}$ ; McCleverty *et al.*, 1980]. The Zn–O bond distances are slightly shorter than those in another zinc acetate complex [ $1.981(2)\text{ \AA}$ ; Razak *et al.*, 2001], and consistent with the interpretation of the coordination as monodentate (Deacon & Phillips, 1980).



**Figure 1**  
The structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

The bond lengths in the 2-aminobenzothiazole ring system (Table 1) are normal, and agree with the corresponding values in a (2-aminobenzothiazole)nitratotin(II) complex (Nardelli *et al.*, 1975). The thiazole planes are almost perpendicular to each other, with a dihedral angle of 80.7 (1)°.

The amino groups lie in their respective attached thiazole planes. It is noteworthy that the two amino groups are not both located on the same side, because of the steric hindrance,



**Figure 2**  
Part of the packing of the title compound, viewed down the *c* direction. Dashed lines indicate hydrogen bonds.

similar to the case of  $\text{Zn}(2\text{-NH}_2\text{py})_2\text{Br}_2$  (Lin *et al.*, 2002). The amino groups of both thiazole ligands are hydrogen bonded to the O atom of the acetate ligands by intramolecular  $\text{N2}\cdots\text{H2A}\cdots\text{O1}$  and  $\text{N4}\cdots\text{H4A}\cdots\text{O3}$  hydrogen bonds. In the crystal, the amino groups also act as donors, to form  $\text{N2}\cdots\text{H2B}\cdots\text{O4}^i$  and  $\text{N4}\cdots\text{H4B}\cdots\text{O2}^{ii}$  hydrogen bonds to acetate O4 and O2 atoms, respectively (Table 2). The  $\text{N2}\cdots\text{H2B}\cdots\text{O4}$  hydrogen bonds interconnect the molecules into chains along the *a* direction, and these are further interconnected into a three dimensional network by  $\text{N4}\cdots\text{H4B}\cdots\text{O2}$  hydrogen bonds (Fig. 2).

Atom Zn1 is also involved in intramolecular interactions with the other O atoms, O2 and O4, from both acetate ligands [ $\text{Zn1}\cdots\text{O2}$  2.795 (3) and  $\text{Zn1}\cdots\text{O4}$  2.692 (3) Å]. These interactions lead to smaller Zn–O–C angles in the title compound [ $\text{Zn1}\text{--O1}\text{--C15}$  113.1 (2) and  $\text{Zn1}\text{--O3}\text{--C17}$  108.3 (2)°] compared with those in the related structure [119.7 (2) and 124.4 (2)°; Razak *et al.*, 2001]. The orientations of the planes of the acetate ligands is nearly orthogonal, the dihedral angle between them being 83.8 (2)°. The Zn1 atom is displaced by 0.029 (1) and 0.276 (1) Å from the acetate planes O1/O2/C15/C16 and O3/O4/C17/C18, respectively.

## Experimental

An ethanolic solution of 2-aminobenzothiazole (4 mmol in 10 ml of ethanol) was added dropwise to  $\text{Zn}(\text{OAc})_2$  (2 mmol in 2 ml of  $\text{H}_2\text{O}$  and 10 ml of ethanol) with stirring. The resulting solution was kept at room temperature. After several days, colorless crystals were obtained and dried under vacuum. Analysis found: C 44.5, H 3.4, S 13.1, N 11.8%; calculated: C 44.7, H 3.7, S 13.3, N 11.6%.

### Crystal data

$[\text{Zn}(\text{C}_2\text{H}_3\text{O}_2)_2(\text{C}_7\text{H}_6\text{N}_2\text{S})_2]$   
 $M_r = 483.89$   
 Orthorhombic,  $Pna2_1$   
 $a = 8.5471$  (7) Å  
 $b = 27.547$  (2) Å  
 $c = 9.0485$  (8) Å  
 $V = 2130.4$  (3) Å<sup>3</sup>  
 $Z = 4$   
 $D_x = 1.509$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation  
 Cell parameters from 7544 reflections  
 $\theta = 2.4\text{--}28.3^\circ$   
 $\mu = 1.38$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Block, colorless  
 0.40 × 0.36 × 0.32 mm

### Data collection

Siemens SMART CCD area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.608$ ,  $T_{\max} = 0.666$   
 12 903 measured reflections

3811 independent reflections  
 3423 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.020$   
 $\theta_{\max} = 28.3^\circ$   
 $h = -11 \rightarrow 11$   
 $k = -36 \rightarrow 33$   
 $l = -7 \rightarrow 12$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.024$   
 $wR(F^2) = 0.060$   
 $S = 1.06$   
 3811 reflections  
 264 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0330P)^2 + 0.1054P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.19$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.23$  e Å<sup>-3</sup>  
 Absolute structure: (Flack, 1983),  
 2485 Friedel pairs  
 Flack parameter = 0.017 (9)

**Table 1**  
Selected geometric parameters (Å).

Zn1—O1	1.960 (2)	S2—C8	1.751 (2)
Zn1—O3	1.968 (2)	N1—C1	1.311 (3)
Zn1—N1	2.034 (2)	N1—C7	1.391 (3)
Zn1—N3	2.039 (2)	N2—C1	1.324 (3)
S1—C2	1.733 (3)	N3—C8	1.317 (3)
S1—C1	1.747 (2)	N3—C14	1.399 (3)
S2—C9	1.749 (3)	N4—C8	1.312 (3)

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

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N2—H2A...O1	0.86	2.05	2.832 (3)	151
N2—H2B...O4 <sup>i</sup>	0.86	1.98	2.824 (3)	168
N4—H4A...O3	0.86	2.10	2.880 (3)	152
N4—H4B...O2 <sup>ii</sup>	0.86	1.98	2.801 (3)	159

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

The H atoms were geometrically fixed and were treated as riding atoms on the parent C and N atoms, with C—H = 0.93–0.96 Å, N—H = 0.86 Å,  $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5U_{\text{eq}}(\text{C})$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$ .

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 1990).

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