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Key indicators

Single-crystal X-ray study
 T = 293 K
 Mean $\sigma(C-C)$ = 0.005 Å
 R factor = 0.036
 wR factor = 0.095
 Data-to-parameter ratio = 16.5

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

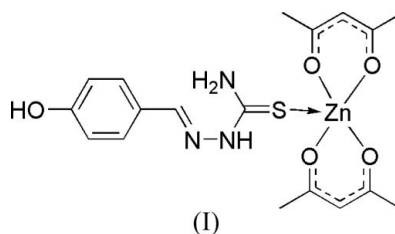
**Bis(acetylacetonato- κ^2O,O')(4-hydroxy-
 benzaldehyde thiosemicarbazone- κS)zinc(II)**

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In the title compound, $[Zn(C_5H_7O_2)_2(C_8H_9N_3OS)]$, the Zn atom has a square-pyramidal coordination formed by four O atoms belonging to two acetylacetonates in the basal square plane and the S atom of the ligand at the apex. The occurrence of N—H···O, N—H···S and O—H···O hydrogen-bonding interactions results in the formation of a layered structure parallel to the (100) plane.

Comment

In recent years, the search for novel molecular chromophores has focused on coordination systems due to their ability to offer a large variety of molecular structures by changing metals, ligands and coordination numbers to enhance thermal stability, and to diverse electronic behaviours by virtue of the coordinated metal center (Long, 1995; Jiang & Fang, 1999; Bella *et al.*, 1995). It has been proved that involvement of metal ions with d^{10} electronic configuration (such as Zn^{2+} , Cd^{2+} and Hg^{2+}) can cause excellent transparency in the visible region, as the metal ions do not form a conjugated system with the ligands and are thus not involved in intramolecular charge transfer (Qin *et al.*, 1999). We report the synthesis and crystal structure of a new zinc(II) coordination compound, (I), with corkscrew-shaped square-pyramidal conformation.



The Zn atom is coordinated by four O atoms of acac groups and one S atom of the HBT (4-hydroxybenzaldehyde thiosemicarbazone) ligand to form a distorted square pyramid (Fig.1). Zn—O distances are 1.996 (2), 2.029 (2), 2.030 (2) and 2.051 (2) Å. The S—Zn bond length is 2.4044 (9) Å while the C11—S1 bond length is 1.717 (3) Å, which is intermediate between a C—S single (1.82 Å) and C=S double (1.56 Å) bond (Duan *et al.*, 1999). The whole molecule can be seen as a corkscrew, in which two acetylacetonato groups form the handles and the HBT group forms the screw.

The occurrence of N—H···O, N—H···S and O—H···O hydrogen-bonding interactions results in the formation of a layered structure parallel to the (100) plane. (Table 1 and Fig. 2).

Experimental

0.193 g (1 mmol) HBT was added to an acetone–acetylacetone (1:1) solution (10 ml) of $(\text{CH}_3)_2\text{COZn}(\text{acac})_2$ (0.33 g, 1 mmol) at 323 K. The mixture was reacted for about 1 h to obtain a yellow precipitate, which was then filtered off and dried under vacuum. (Yield 0.30 g, 65%). Single crystals suitable for X-ray crystal structure analysis were obtained by slow evaporation of an acetoneacetyl (1:1) solution in air.

Crystal data

$[\text{Zn}(\text{C}_5\text{H}_7\text{O}_2)_2(\text{C}_8\text{H}_9\text{N}_3\text{OS})]$
 $M_r = 458.82$
 Orthorhombic, *Pbca*
 $a = 14.3048$ (7) Å
 $b = 10.1746$ (5) Å
 $c = 29.7259$ (15) Å
 $V = 4326.5$ (4) Å³

$Z = 8$
 $D_x = 1.409$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 1.26$ mm⁻¹
 $T = 293$ (2) K
 Block, colorless
 $0.48 \times 0.41 \times 0.39$ mm

Data collection

Bruker SMART 1000 CCD
 diffractometer
 ω scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.559$, $T_{\max} = 0.613$

20382 measured reflections
 4266 independent reflections
 2782 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.042$
 $\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.095$
 $S = 1.04$
 4266 reflections
 258 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2 + 3.1381P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.005$
 $\Delta\rho_{\text{max}} = 0.49$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.25$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O5}-\text{H5}\cdots\text{O1}^{\text{i}}$	0.82	1.95	2.742 (3)	162
$\text{N2}-\text{H2}\cdots\text{S1}^{\text{ii}}$	0.86	2.57	3.422 (3)	171
$\text{N1}-\text{H1E}\cdots\text{O2}$	0.86	1.96	2.805 (3)	169
$\text{N1}-\text{H1D}\cdots\text{O4}^{\text{iii}}$	0.86	2.16	2.926 (3)	149

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

All the H atoms were placed in geometrically idealized positions ($C-H = 0.96$ Å) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT-Plus (Bruker, 2003); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXTL (Bruker, 2005); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

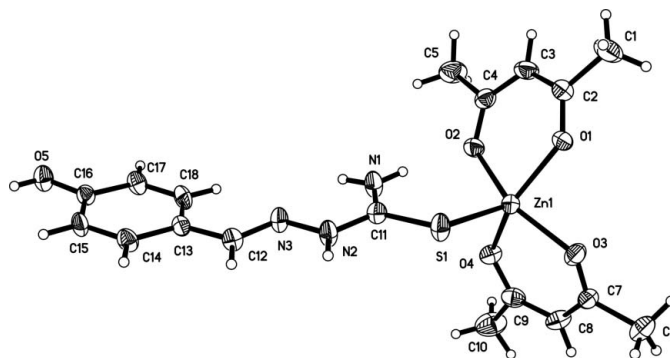


Figure 1

The molecular structure of the title compound with the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as spheres of arbitrary radii.

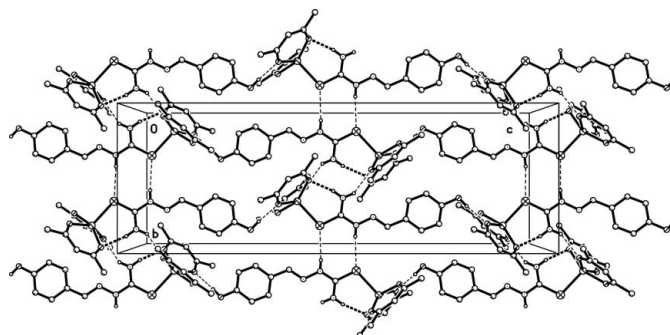


Figure 2

Crystal packing of the title compound, showing the hydrogen-bonding network. Hydrogen bonds are represented as dashed lines. H atoms not involved in hydrogen bonds have been omitted for clarity.

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