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Key indicators

Single-crystal X-ray study T = 293 K Mean σ (C–C) = 0.006 Å Disorder in main residue R factor = 0.052 wR factor = 0.149 Data-to-parameter ratio = 15.5

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

(Dimethyl sulfoxide-κS)bis[2'-(3-methylthiophen-2-ylmethylene)furan-2-carbohydrazido]zinc(II)

The title compound, $[Zn(C_{12}H_{10}N_2O_2S)_2(C_2H_6OS)]$, is monomeric with the Zn atom in a five-coordinate environment. The geometry of the polyhedron is distorted trigonal bipyramidal, with angles of the equatorial atoms about the central Zn atom in the range 77.84 (10)–126.66 (12) Å. The O–Zn–O axial bond angle is 173.12 (12)°.

Comment

The title compound, (I), is an example of the coordination of a dimethyl sulfoxide (DMSO) solvent molecule to the Zn atom when $[Zn(C_{12}H_{10}N_2O_2S)_2]$ was recrystallized from DMSO. The central Zn atom is chelated in a bidentate manner by the ligands via atoms O1, N2, O4 and N4 and in monodentate fashion by atom O3 of the DMSO molecule, forming a fivecoordinate environment. The geometry of the central Zn atom is distorted trigonal bipyramidal, with atoms O1 and O4 occupying the axial positions at an angle of 173.12 (12)° about the Zn atom. Atoms Zn1, N2, N4 and O3, occupying the equatorial positions, are coplanar, with a maximum displacement of 0.003 (1) Å from the mean plane for Zn1. The axial Zn-O distances [2.038 (2) and 2.045 (2) Å] are slightly longer than the equatorial Zn1-O3 distance of 1.997 (3) Å, and the Zn-N distances of 2.027 (3) and 2.025 (3) Å are in agreement with other five-coordinate Zn complexes, such as $[Zn_2(C_{15}H_{12}N_2O_2)_2(C_2H_6OS)_2]$, where average Zn-O and Zn-N bonds are 2.02 (2) and 2.047 (2) Å, respectively (Ali et al., 2003).



The structural dimensions of the chelating ligands are typical for Schiff bases and in normal ranges (Orpen *et al.*, 1989; Allen *et al.*, 1987). The chelating O1/C1/C5/N1/N2 [maximum deviation -0.014 (1) Å for O1] and O4/C16/N3/N4 [maximum deviation 0.053 (3) Å for N4] moieties are planar and inclined by 51.46 (13)° to each other. The thiophene fragments, S1/C7/C8/C9/C10 and S2/C18/C19/C20/C21, make a dihedral angle of 52.0 (2)°. The furyl fragments, C1/C2/C3/O2/C4 and C12/C13/C14/C15/O5, are inclined to each other by 49.2 (3)°.

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View of (I), with 50% probability displacement ellipsoids. Only the major component (S3A) of disordered atom S3 is shown.

In the crystal structure, the molecules are linked by intermolecular interactions $C1-H1B\cdots O1^{i}$ to form polymeric chains parallel to the *a* axis and C20–H20A···O4ⁱⁱ (symmetry codes as in Table 2) connecting pairs of molecules in the chain to form dimeric units (Fig. 2).

Experimental

To a stirred methanol solution (75 ml) of 2-furoic acid hydrazide (2.5 g, 20 mmol), 3-methyl-2-thiophenecarboxaldehyde (2.1 ml, 20 mmol) and triethylamine (2.8 ml, 20 mmol) were added dropwise. Zinc(II) acetate dihydrate (2.2 g, 10 mmol) in methanol (100 ml) was added and the mixture was refluxed for 5 h. The resulting solution was filtered from the dark brown precipitate and the clear-yellow solution was reduced to one-third of its volume. On cooling, a yellowbrown solid was obtained, washed with methanol and diethyl ether and recrystallized from DMSO.

Crystal data

$[Zn(C_{12}H_{10}N_2O_2S)_2(C_2H_6OS)]$	Z = 2
$M_r = 610.02$	$D_x = 1.470 \text{ Mg m}^{-3}$
Triclinic, P1	Mo $K\alpha$ radiation
a = 10.4060 (19) Å	Cell parameters from 5500
b = 10.640 (2) Å	reflections
c = 13.152 (2) Å	$\theta = 1.5 - 26.0^{\circ}$
$\alpha = 93.067 \ (4)^{\circ}$	$\mu = 1.16 \text{ mm}^{-1}$
$\beta = 98.772 \ (4)^{\circ}$	T = 293 (2) K
$\gamma = 105.796 \ (4)^{\circ}$	Block, yellow
V = 1377.9 (4) Å ³	$0.34 \times 0.28 \times 0.10 \text{ mm}$
Data collection	
Bruker SMART APEX CCD area-	5322 independent reflections
detector diffractometer	4164 reflections with $I > 2\sigma(I)$
ω scans	$R_{\rm int} = 0.026$
Absorption correction: multi-scan	$\theta_{\rm max} = 26.0^{\circ}$
(SADABS; Sheldrick, 1996)	$h = -12 \rightarrow 9$
$T_{\min} = 0.693, \ T_{\max} = 0.892$	$k = -13 \rightarrow 13$
10224 measured reflections	$l = -16 \rightarrow 16$



Packing diagram of (I). The dashed lines denote $C-H\cdots O$ hydrogen bonds.

constrained

Refinement

Refinement on F^2	H-atom parameters constrai		
$R[F^2 > 2\sigma(F^2)] = 0.052$	$w = 1/[\sigma^2 (F_o^2) + (0.0898P)^2]$		
$wR(F^2) = 0.149$	where $P = (F_o^2 + 2F_c^2)/3$		
S = 1.04	$(\Delta/\sigma)_{\rm max} < 0.001$		
5322 reflections	$\Delta \rho_{\rm max} = 0.56 \text{ e } \text{\AA}^{-3}$		
344 parameters	$\Delta \rho_{\rm min} = -0.34 \text{ e } \text{\AA}^{-3}$		

Table 1

Selected geometric parameters (Å, °).

Zn1-O3	1.997 (3)	O2-C4	1.362 (4)
Zn1-N4	2.022 (3)	O4-C16	1.266 (4)
Zn1-N2	2.032 (3)	O5-C13	1.346 (6)
Zn1-O4	2.038 (2)	O5-C15	1.346 (5)
Zn1-O1	2.045 (2)	N1-C5	1.306 (4)
S1-C8	1.693 (4)	N1-N2	1.374 (4)
S1-C7	1.730 (4)	N2-C6	1.283 (4)
S2-C19	1.699 (5)	N3-C16	1.321 (4)
S2-C18	1.716 (4)	N3-N4	1.370 (4)
O1-C5	1.271 (4)	N4-C17	1.285 (4)
O2-C3	1.352 (5)		
O3-Zn1-N4	115.33 (12)	O3-Zn1-O1	96.51 (12)
O3-Zn1-N2	118.01 (13)	N4-Zn1-O1	96.89 (11)
N4-Zn1-N2	126.66 (12)	N2-Zn1-O1	77.84 (10)
O3-Zn1-O4	89.96 (12)	O4-Zn1-O1	173.12 (10)
N4-Zn1-O4	78.15 (10)	C8-S1-C7	91.4 (2)
N2-Zn1-O4	101.19 (10)		

Table 2

Hydrogen-bonding geometry (Å, °).

$D - H \cdot \cdot \cdot A$	$D-\mathrm{H}$	$H \cdot \cdot \cdot A$	$D \cdot \cdot \cdot A$	$D - \mathbf{H} \cdots A$
$\begin{array}{c} C1 - H1B \cdots O1^{i} \\ C20 - H20A \cdots O4^{ii} \end{array}$	0.93	2.50	3.385 (5)	159
	0.93	2.46	3.308 (5)	152

Symmetry codes: (i) -x, 1 - y, -z; (ii) x - 1, y, z.

After their location in a difference map, all H atoms were positioned geometrically and allowed to ride on their parent C atoms with C-H = 0.93-0.96 Å and $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C)$, respectively. S1 and the methyl H atoms at C23 and C24 are clearly disordered and each group was modelled using alternative sites of half-occupancy.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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