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catena-Poly[[[4-bromo-2-(2-dimethylaminoethyliminomethyl)phenolato]zinc(II)]-μ-thiocyanato]

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.008 Å
R factor = 0.041
wR factor = 0.093
Data-to-parameter ratio = 18.3

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

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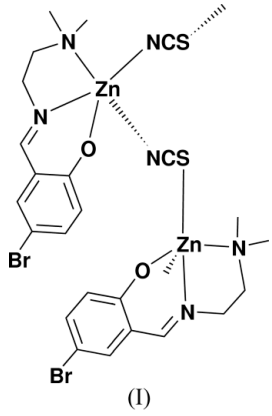
The title Schiff base compound, $[Zn(C_{11}H_{14}N_2O)(NCS)]_n$, crystallizes with two independent molecules in the asymmetric unit. The Zn^{II} atoms are five-coordinated by two N atoms and one O atom from a Schiff base ligand, one N atom from a thiocyanate anion and one S atom from another thiocyanate anion of a symmetry-related molecule. This gives rise to the formation of zigzag polymeric chains with a $[-Zn-N-C-S-Zn-]_n$ backbone running along the a axis.

Comment

Zinc(II) has long been recognized as a structural template in protein folding or as a Lewis acid catalyst that can readily adopt four-, five- or six-coordination (Vallee & Auld, 1993; Lipscomb & Sträter, 1996). As an extension of work on the structural characterization of zinc complexes, the title mononuclear zinc(II) compound, (I), is reported here.



(I)

Compound (I) is an electronically neutral mononuclear zinc(II) compound (Fig. 1). The asymmetric unit contains two independent molecules. In both molecules, the Zn^{II} atoms are in a square-pyramidal geometry and are five-coordinated by two N atoms and one O atom from a Schiff base ligand, one N atom from a thiocyanate anion and one S atom from another thiocyanate anion of a symmetry-related molecule. The four coordinating atoms in the basal planes around the Zn centers are approximately coplanar, with an average deviation of 0.015 (8) Å for Zn1 and 0.018 (8) Å for Zn2; the Zn1 and Zn2 atoms lie, respectively, 0.179 (3) and 0.182 (3) Å above the corresponding planes. The average Zn—O bond lengths [1.918 (3) Å for Zn1 and 1.921 (4) Å for Zn2; Table 1] are a little longer than the corresponding values observed in a Schiff base zinc(II) complex described previously (You *et al.*, 2003). The Zn—N(imine) bond lengths [1.944 (4) Å for Zn1 and 1.947 (4) Å for Zn2] are a little shorter than the values observed in the complex cited above. The pyramidal Zn—S

distances are 2.827 (16) Å for Zn1—S1^{i} and 2.828 (15) Å for Zn2—S2^{ii} (see Table 1 for symmetry codes).

In the crystal structure, the independent complexes form polymers extending in the *a*-axis direction (Fig. 2). There are weak C—H···O hydrogen bonds in the crystal structure (Table 2).

Experimental

5-Bromosalicylaldehyde (0.1 mmol, 20.1 mg), *N,N*-dimethylethane-1,2-diamine (0.1 mmol, 8.8 mg), ammonium thiocyanate (0.1 mmol, 7.6 mg) and $Zn(CH_3COO)_2{\cdot}2H_2O$ (0.1 mmol, 22.0 mg) were dissolved in methanol (10 ml). The mixture was stirred at room temperature for 1 h to give a clear yellow solution. After keeping the solution in air for 11 d, yellow block-shaped crystals were formed.

Crystal data

$[Zn(C_{11}H_{14}N_2O)(NCS)]$
M_r = 393.60
Orthorhombic, $Pca2_1$
a = 11.750 (2) Å
b = 7.410 (2) Å
c = 33.842 (7) Å
V = 2946.7 (10) Å^3
Z = 8
D_x = 1.774 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6908 reflections
θ = 2.5–24.8°
μ = 4.52 mm^{-1}
T = 298 (2) K
Block, yellow
0.22 × 0.13 × 0.11 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.437, T_{max} = 0.637
30314 measured reflections
6356 independent reflections
5330 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 27.5°
$h = -15 \rightarrow 15$
$k = -9 \rightarrow 9$
$l = -35 \rightarrow 35$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.093
S = 1.07
6356 reflections
347 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0226P)^2 + 2.4441P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.09 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Absolute structure: Flack (1983); 2912 Friedel pairs
Flack parameter = 0.056 (11)

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.918 (3)	Zn2—O2	1.921 (4)
Zn1—N1	1.944 (4)	Zn2—N4	1.947 (4)
Zn1—N3	1.952 (4)	Zn2—N6	1.966 (4)
Zn1—N2	2.066 (4)	Zn2—N5	2.064 (4)
Zn1—S1^{i}	2.8271 (16)	Zn2—S2^{ii}	2.8288 (15)
O1—Zn1—N1	92.26 (16)	O2—Zn2—N4	91.67 (16)
O1—Zn1—N3	90.46 (17)	O2—Zn2—N6	90.00 (17)
N1—Zn1—N3	168.0 (2)	N4—Zn2—N6	168.0 (2)
O1—Zn1—N2	170.12 (18)	O2—Zn2—N5	170.29 (18)
N1—Zn1—N2	83.89 (17)	N4—Zn2—N5	85.22 (17)
N3—Zn1—N2	91.52 (17)	N6—Zn2—N5	91.18 (17)
O1—Zn1—S1^{i}	97.78 (13)	O2—Zn2—S2^{ii}	97.87 (13)
N1—Zn1—S1^{i}	90.31 (12)	N4—Zn2—S2^{ii}	89.78 (12)
N3—Zn1—S1^{i}	100.91 (16)	N6—Zn2—S2^{ii}	101.78 (16)
N2—Zn1—S1^{i}	91.35 (13)	N5—Zn2—S2^{ii}	91.32 (12)

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

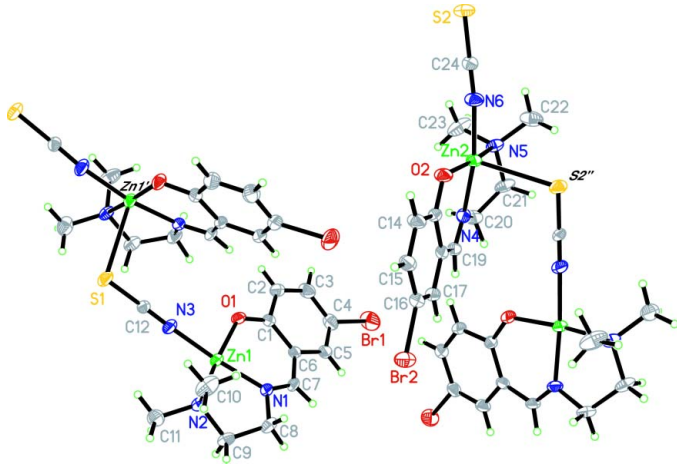


Figure 1
The structure of the asymmetric unit of (I), together with symmetry-generated units to show the polymeric chain connections. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented by small spheres. [Symmetry codes: (') $\frac{1}{2}+x, 1-y, z$; ('') $\frac{1}{2}+x, 2-y, z$.]

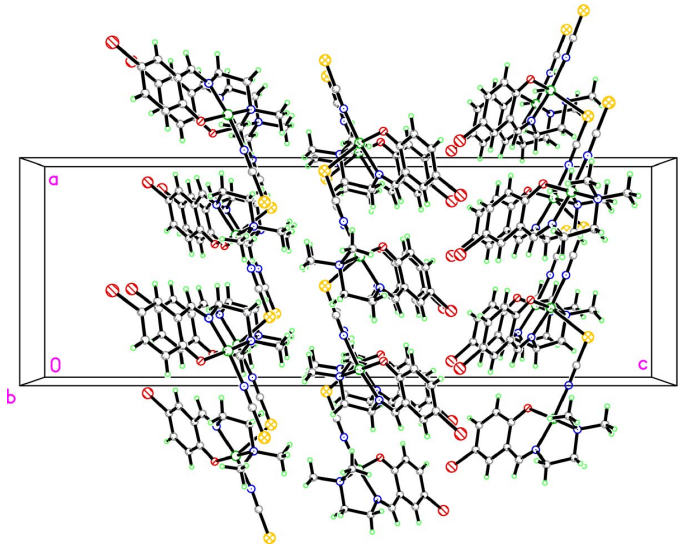


Figure 2
The crystal packing of (I), viewed along the *b* axis.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O1^{i}	0.93	2.51	3.285 (7)	141
C19—H19···O2^{ii}	0.93	2.55	3.308 (7)	139
C20—H20*B*···O2^{ii}	0.97	2.58	3.468 (7)	153

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

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2 or 1.5U_{eq}(C). An unassigned maximum residual density of 1.09 e Å^{-3} was observed 0.85 Å from atom Br1.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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*.

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