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catena-Poly[[[aquazinc(II)]-μ-2,2′-dithiodibenzoato] bis(*N*,*N*-dimethylformamide)]

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Key indicators

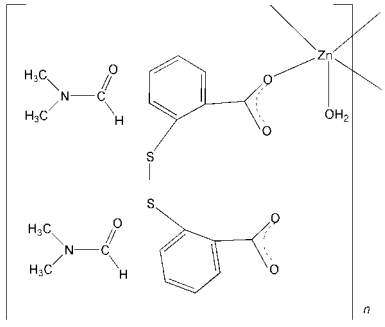
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.054
wR factor = 0.125
Data-to-parameter ratio = 14.0

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

In the title compound, $\{[Zn(C_{14}H_8O_4S_2)(H_2O)]\cdot 2C_3H_7NO\}_n$, the 2,2′-dithiodibenzenecarboxylate anion, which acts as a bridge, is tetradentate to water-coordinated zinc(II) ions, forming a polymeric double-chain ribbon. The geometry around the zinc(II) ion is that of a square pyramid. The coordinated water molecules and uncoordinated *N*,*N*-dimethylformamide molecules are linked by hydrogen bonds.

Comment

The 2,2′-dithiodibenzenecarboxylate (dtbc) anion binds to metal atoms in a variety of bonding modes, and two of its complexes have been structurally characterized (Ganesh *et al.*, 1990; Toby *et al.*, 1981). These studies have been extended to the present polymeric zinc complex, (I), in which each dtbc anion functions as a bridge linking four zinc ions.



(I)

In (I), each zinc ion is coordinated by four O atoms from four carboxylate groups of four dtbc anions, with a typical Zn—O(carboxylate) distance range [2.041 (3)–2.056 (3) Å; Chen *et al.*, 1994] and one water molecule, with a shorter Zn—O distance [1.964 (3) Å], resulting in a slightly distorted square-pyramidal coordination polyhedron (Table 1 and Fig. 1). The square plane containing atoms O3, O2^{i}, O4^{ii} and O1^{iii} [symmetry codes: (i) $-x+1, -y+2, -z$; (ii) $-x, -y+2, -z$; (iii) $x-1, y, z$; mean deviation 0.0028 Å] is slightly distorted. Four carboxylate groups bridge two zinc ions, forming centrosymmetric binuclear units with Zn···Zn separations of 2.9978 (8) Å, and a dihedral angle of 76.5 (1)° between the planes through the two aromatic rings. The dtbc anions link the binuclear units, generating a polymeric double-chain ribbon (Fig. 2). The *N*,*N*-dimethylformamide molecules are involved in hydrogen-bonding interactions with the coordinated water molecule (Table 2).

Experimental

A solution (10 ml) of ethanol containing 2,2′-dithiodibenzoic acid (0.33 mmol, 0.10 g) was added slowly to a dimethylformamide solu-

tion (10 ml) of zinc dimethyldithiocarbamate (0.5 mmol, 0.04 g). The mixture was stirred for a few minutes and left to stand at room temperature for a week, affording colorless block-shaped crystals.

Crystal data

$[Zn(C_{14}H_8O_4S_2)(H_2O)]\cdot 2C_3H_7NO$
$M_r = 533.90$
Monoclinic, $P2_1/c$
$a = 11.0956$ (4) Å
$b = 17.2715$ (7) Å
$c = 12.2400$ (5) Å
$\beta = 95.695$ (2)°
$V = 2334.07$ (16) Å^3
$Z = 4$
$D_x = 1.519$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2880 reflections
$\theta = 2.4$–26.6°
$\mu = 1.27$ mm^{-1}
$T = 298$ (2) K
Block, colorless
0.46 × 0.18 × 0.10 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.592$, $T_{max} = 0.883$
12 296 measured reflections
4193 independent reflections
3417 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 25.2°$
$h = -13 \rightarrow 12$
$k = -20 \rightarrow 20$
$l = -13 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.125$
$S = 1.08$
4193 reflections
299 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0625P)^2 + 1.0746P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.70$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O7	1.960 (3)	Zn1—O4^{ii}	2.044 (3)
Zn1—O3	2.041 (3)	Zn1—O1^{iii}	2.056 (3)
Zn1—O2^{i}	2.042 (2)	Zn1···Zn1^{ii}	2.9979 (8)
O7—Zn1—O3	101.68 (12)	O2^{i}—Zn1—O4^{ii}	87.27 (12)
O7—Zn1—O2^{i}	103.34 (12)	O7—Zn1—O1^{iii}	98.11 (12)
O3—Zn1—O2^{i}	89.36 (12)	O3—Zn1—O1^{iii}	87.44 (12)
O7—Zn1—O4^{ii}	100.13 (13)	O2^{i}—Zn1—O1^{iii}	158.51 (11)
O3—Zn1—O4^{ii}	158.12 (11)	O4^{ii}—Zn1—O1^{iii}	87.83 (12)
C1—S1—S2—C8	−96.55 (18)		

Symmetry codes: (i) $1-x, 2-y, -z$; (ii) $-x, 2-y, -z$; (iii) $x-1, y, z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7A···O5^{iv}	0.840 (19)	1.79 (2)	2.613 (5)	166 (5)
O7—H7B···O6^{iii}	0.841 (19)	1.78 (2)	2.619 (4)	172 (5)
C2—H2···S2	0.93	2.74	3.220 (4)	113
C5—H5···O1	0.93	2.51	2.796 (5)	98
C9—H9···S1	0.93	2.75	3.216 (4)	112
C12—H12···O4	0.93	2.50	2.788 (5)	98
C15—H15A···O5	0.96	2.48	2.820 (11)	101
C19—H19A···O6	0.96	2.35	2.761 (8)	105

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

Water H atoms were refined [O—H = 0.840 (19) and 0.841 (19) Å]. All other H atoms were positioned geometrically and allowed to ride on their parent atoms at Csp^2—H distances of 0.93 Å, with U_{iso}(H) = 1.2U_{eq}(parent atom), and Csp^3—H distances of 0.96 Å, with U_{iso}(H) = 1.5U_{eq}(parent atom).

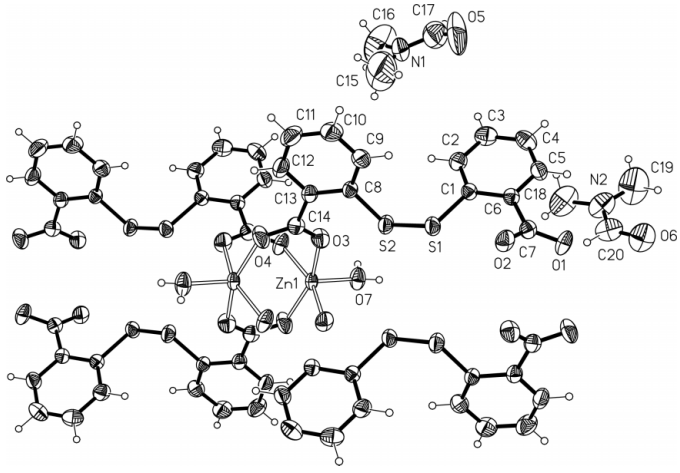


Figure 1
Part of the polymeric structure of (I), with the atom-numbering scheme for the asymmetric unit, and displacement ellipsoids shown at the 50% probability level.

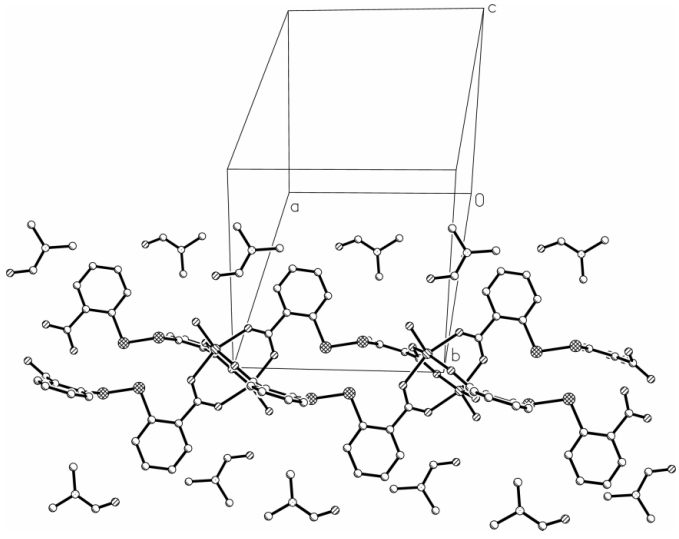


Figure 2
The polymeric double chain of (I). H atoms have been omitted for clarity.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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