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Bis(μ-piperidine-1-dithiocarboxylato-κ^2S:S')-[bis(piperidine-1-dithiocarboxylato-κ^2S,S')zinc(II)]

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Key indicators

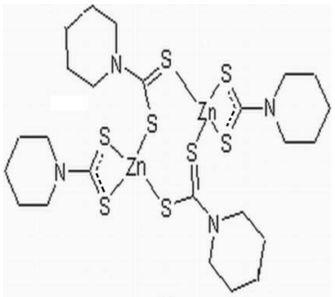
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.034
wR factor = 0.079
Data-to-parameter ratio = 16.9

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

In the title compound, $[Zn_2(C_6H_{10}NS_2)_4]$, the Zn atom is tetrahedrally coordinated by one *S*,*S*′-bidentate and two *S*-monodentate dithiocarbamate ligands. The monodentate ligands also bridge to a second Zn atom, resulting in a metallacyclic dimer, generated by inversion symmetry.

Comment

A number of centrosymmetric dimeric zinc(II)–dithiocarbamate complexes have been reported involving ligands such as ethylisopropyldithiocarbamate (Baba *et al.*, 2001*a*) or ethylbutyldithiocarbamate (Baba *et al.*, 2001*b*). The dimeric title complex, (I) (Fig. 1), represents another member of this family of compounds.



(I)

In (I), the center of gravity coincides with a center of symmetry. The C1-containing dithiocarbamate group behaves as a chelating bidentate ligand with comparable Zn—S bond lengths (Table 1) coordinating through atoms S1 and S2. The second dithiocarbamate anion bridges two adjacent Zn atoms through atoms S3 and S4, giving a centrosymmetric dimer. The coordination geometry about the Zn atom is distorted tetrahedral (Table 1), with the S1—Zn1—S2 bond angle substantially compressed. The C—S bond lengths in (I) suggest that the negative charge of the C1/S1/S2 group is delocalized, while that of the C7/S3/S4 group is essentially localized.

The unit-cell packing for (I) is shown in Fig. 2.

Experimental

Carbon disulfide (0.75 g, 9.85 mmol, Aldrich) was added to an ethanolic solution (25 ml) of piperidine (0.838 g, 9.85 mmol, Aldrich) with constant stirring at 273 K. After 2 h, an ethanolic solution (10 ml) of zinc chloride (0.322 g, 4.925 mmol) was added. The mixture was stirred vigorously and set aside. The solid was isolated, washed with an excess of ethanol and recrystallized from a dichloromethane–methanol (1:1) mixture as colourless plates.

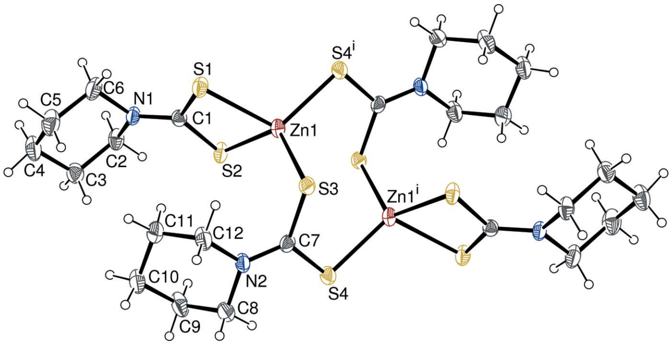


Figure 1
The structure of (I), showing the atom-numbering scheme, with displacement ellipsoids drawn at the 50% probability level. [Symmetry code: (i) $-x$, $2 - y$, $-z$.]

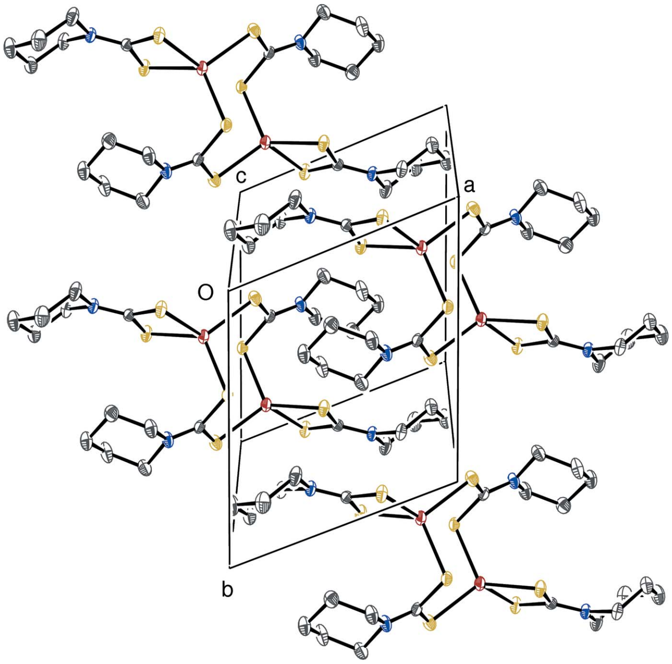


Figure 2
The arrangement of molecules of (I) in the unit cell. H atoms have been omitted for clarity.

Crystal data

$[Zn_2(C_6H_{10}NS_2)_4]$
$M_r = 771.83$
Triclinic, $P\bar{1}$
$a = 8.7109$ (19) Å
$b = 9.624$ (2) Å
$c = 11.3166$ (16) Å
$\alpha = 103.343$ (17)°
$\beta = 97.502$ (15)°
$\gamma = 112.87$ (2)°
$V = 824.5$ (3) Å^3
$Z = 1$
$D_x = 1.554$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.98$ mm^{-1}
$T = 293$ (2) K
Plate, colourless
0.25 × 0.16 × 0.03 mm

Data collection

Oxford Diffraction Xcalibur2 CCD diffractometer
$\omega/2\theta$ scans
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2004)
$T_{min} = 0.644$, $T_{max} = 0.915$
5594 measured reflections
2913 independent reflections
1918 reflections with $I > 2s\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 25.1°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.079$
$S = 0.93$
2913 reflections
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0367P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—S4^i	2.3240 (11)	C1—S1	1.727 (3)
Zn1—S2	2.3256 (11)	C1—S2	1.734 (3)
Zn1—S3	2.3722 (12)	C7—S3	1.753 (3)
Zn1—S1	2.4712 (13)	C7—S4	1.716 (3)
S4^i—Zn1—S2	129.05 (4)	S4^i—Zn1—S1	109.75 (4)
S4^i—Zn1—S3	105.56 (4)	S2—Zn1—S1	75.86 (4)
S2—Zn1—S3	120.12 (4)	S3—Zn1—S1	110.18 (4)

Symmetry code: (i) $-x + 2$, $-y + 1$, $-z + 1$.

All H atoms were placed in idealized positions (C—H = 0.97 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *CrysAlis RED* (Oxford Diffraction, 2004); cell refinement: *CrysAlis RED*; data reduction: *CrysAlis RED*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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Acta Cryst. (2006). E**62**, m1186–m1187 Shaheen *et al.* • $[Zn_2(C_6H_{10}NS_2)_4]$ **m1187**