

Bis(μ -4-methylpiperidine-1-dithiocarboxylato- κ^2 S:S')-[bis(4-methylpiperidine-1-dithiocarboxylato-S:S')-zinc(II)]

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Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.006\text{ \AA}$
 R factor = 0.043
 wR factor = 0.124
Data-to-parameter ratio = 23.3

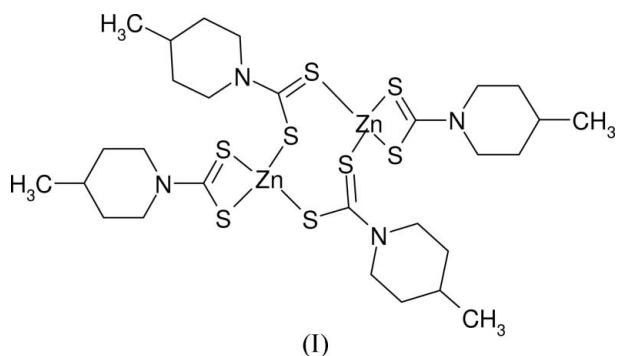
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the centrosymmetric title compound, $[\text{Zn}_2(\text{C}_7\text{H}_{12}\text{NS}_2)_4]$, each Zn atom is chelated by one dithiocarboxylate group, while the other dithiocarboxylate ligand bridges the two Zn atoms to form a dimeric binuclear complex. The coordination geometry about each Zn atom is distorted tetrahedral.

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Comment

The structure of zinc(II) dithiocarbamate is that of a centrosymmetric dimer (Cox & Tiekkink, 1997). Zinc dithiocarbamates have been studied as antioxidant additives to photographic film (Fukumoto *et al.*, 1986) and as hydrocarbon-based lubricants (Shelkova *et al.*, 1990). A number of other centrosymmetric dimeric zinc(II) dithiocarbamate complexes have been reported, such as the ethyl isopropylidethiocarbamate complex (Baba *et al.*, 2001a) and the ethyl butylidethiocarbamate complex (Baba *et al.*, 2001b).



In the title complex, (I), the asymmetric unit contains one-half of the complex molecule, which lies about a centre of symmetry. One dithiocarboxylate group behaves as a chelating bidentate ligand, coordinating through atoms S3 and S4, while

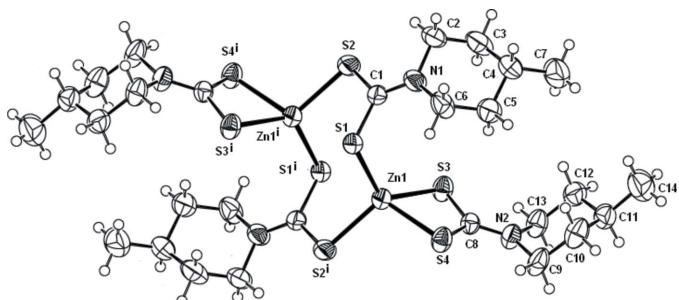


Figure 1

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

the other bidentate dithiocarboxylate ligand bridges two adjacent Zn atoms through atoms S1 and S2ⁱ [symmetry code: (i) $-x, 2 - y, -z$] to give a centrosymmetric dimer (Fig. 1). The coordination geometry about the Zn atoms is distorted tetrahedral (Table 1).

Experimental

Carbon disulfide (0.55 g, 7.34 mmol) was added to an ethanolic solution of 4-methylpiperidine (0.72 g, 7.34 mmol) with constant stirring at 273 K. After 2 h, an ethanolic solution of zinc chloride (0.50 g, 3.67 mmol) was added. The mixture was stirred vigorously and set aside. The solid which formed was isolated, washed with an excess of ethanol and recrystallized from a dichloromethane–methanol (1:1) mixture.

Crystal data

$[\text{Zn}_2(\text{C}_7\text{H}_{12}\text{NS}_2)_4]$	$Z = 1$
$M_r = 827.92$	$D_x = 1.438 \text{ Mg m}^{-3}$
Triclinic, $\bar{P}\bar{1}$	Mo $K\alpha$ radiation
$a = 8.1806 (10) \text{ \AA}$	Cell parameters from 194 reflections
$b = 11.4347 (11) \text{ \AA}$	$\theta = 4.2\text{--}29.4^\circ$
$c = 11.9679 (12) \text{ \AA}$	$\mu = 1.72 \text{ mm}^{-1}$
$\alpha = 108.808 (9)^\circ$	$T = 293 (2) \text{ K}$
$\beta = 107.280 (10)^\circ$	Prism, colourless
$\gamma = 101.583 (9)^\circ$	$0.3 \times 0.2 \times 0.15 \text{ mm}$
$V = 955.9 (2) \text{ \AA}^3$	

Data collection

Oxford Diffraction Xcalibur2 CCD diffractometer
 $\omega/2\theta$ scans
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2004)
 $T_{\min} = 0.450$, $T_{\max} = 0.819$
7446 measured reflections

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.124$
 $S = 1.06$
4480 reflections
192 parameters
H-atom parameters constrained

4480 independent reflections
3095 reflections with $I > 2s\sigma(I)$
 $R_{\text{int}} = 0.020$
 $\theta_{\text{max}} = 28.3^\circ$
 $h = -10 \rightarrow 10$
 $k = -15 \rightarrow 14$
 $l = -13 \rightarrow 15$

$$w = 1/[\sigma^2(F_o^2) + (0.0674P)^2 + 0.1131P]$$

where $P = (F_o^2 + 2F_c^2)/3$

$$(\Delta/\sigma)_{\text{max}} < 0.001$$

$$\Delta\rho_{\text{max}} = 0.61 \text{ e \AA}^{-3}$$

$$\Delta\rho_{\text{min}} = -0.34 \text{ e \AA}^{-3}$$

Table 1
Selected geometric parameters (\AA , $^\circ$).

Zn1–S1	2.3552 (9)	S4–C8	1.713 (3)
Zn1–S2 ⁱ	2.3277 (10)	N1–C1	1.310 (4)
Zn1–S3	2.3366 (9)	N1–C6	1.473 (4)
Zn1–S4	2.4630 (9)	N1–C2	1.483 (4)
S1–C1	1.751 (3)	N2–C8	1.318 (4)
S2–C1	1.722 (3)	N2–C9	1.476 (4)
S3–C8	1.739 (3)	N2–C13	1.470 (4)
S2 ⁱ –Zn1–S1	106.06 (4)	S3–Zn1–S4	75.62 (3)
S3–Zn1–S1	124.13 (4)	S1–Zn1–S4	110.52 (3)
S2 ⁱ –Zn1–S3	126.10 (4)		

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

All H atoms were refined using a riding model, with C–H = 0.93 \AA and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aromatic H, C–H = 0.97 \AA and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for CH_2 , and C–H = 0.96 \AA and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for CH_3 .

Data collection: *CrysAlis CCD* (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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