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Key indicators

Single-crystal X-ray study
T = 298 K
Mean $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$
R factor = 0.047
wR factor = 0.114
Data-to-parameter ratio = 21.2

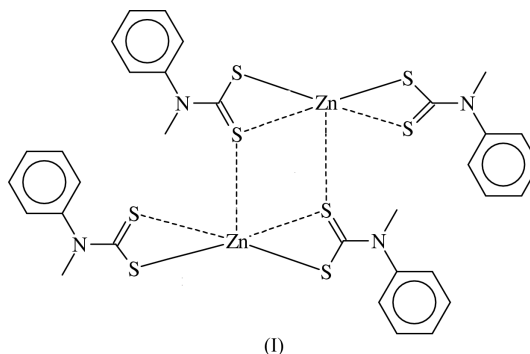
For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

Bis(μ -N-methyl-N-phenyldithiocarbamato)- [bis(N-methyl-N-phenyldithiocarbamato)zinc(II)]

The Zn atom in the centrosymmetric title compound, $[\text{Zn}_2(\text{C}_8\text{H}_8\text{NS}_2)_4]$, is almost symmetrically coordinated by one terminal bidentate N-phenyl-N-methyldithiocarbamate ligand [$\text{Zn}-\text{S}$ 2.348 (1) and 2.459 (1) \AA] and non-symmetrically coordinated by a second bidentate bridging dithiocarbamate ligand [$\text{Zn}-\text{S}$ 2.316 (1) and 2.980 (1) \AA]. The latter also uses its bridging S atom to coordinate the second Zn atom [$\text{Zn}-\text{S}$ 2.378 (1) \AA], thus forming a dimeric binuclear complex. Taking into account the long $\text{Zn}\cdots\text{S}$ distance, the Zn atom has a distorted trigonal-bipyramidal coordination.

Comment

The crystal structures of a number of zinc(II) dithiocarbamates have been reported; such compounds exist as centrosymmetric dimers (Cox & Tiekink, 1997). We have previously described complexes with ethylisopropyldithiocarbamate (Baba *et al.*, 2001a), as well as ethylbutyldithiocarbamate (Baba *et al.*, 2001b) ligands.



In the title compound, (I) (Fig. 1), both dithiocarbamate groups chelate to the Zn atom. One of the dithiocarbamates represents a terminal bidentate ligand with comparable bond lengths [$\text{Zn1}-\text{S3}$ 2.348 (1) \AA and $\text{Zn1}-\text{S4}$ 2.459 (1) \AA]. Another dithiocarbamate coordinates the Zn atom in a bridging bidentate manner, forming two distinctly unequal $\text{Zn1}-\text{S1}$ and $\text{Zn1}\cdots\text{S2}$ bonds [2.316 (1) and 2.980 (1) \AA , respectively]. The C-S bonds in both of the ligands are delocalized and can hardly be distinguished formally as single or double bonds [$\text{C1}-\text{S3}$ 1.732 (3), $\text{C1}-\text{S4}$ 1.712 (3), $\text{C9}-\text{S1}$ 1.717 (2) and $\text{C9}-\text{S2}$ 1.742 (2) \AA]. Atom S2, which forms the longer C-S bond in the bridging ligand, interacts across the inversion center with an adjacent Zn atom, forming a short $\text{S2}-\text{Zn1}^i$ bond [2.378 (1) \AA ; symmetry code: (i) $1-x, 1-y, 1-z$]. If the long $\text{Zn1}\cdots\text{S2}$ interaction is taken into account, the coordination geometry of Zn1 may be described as a severely distorted trigonal bipyramid.

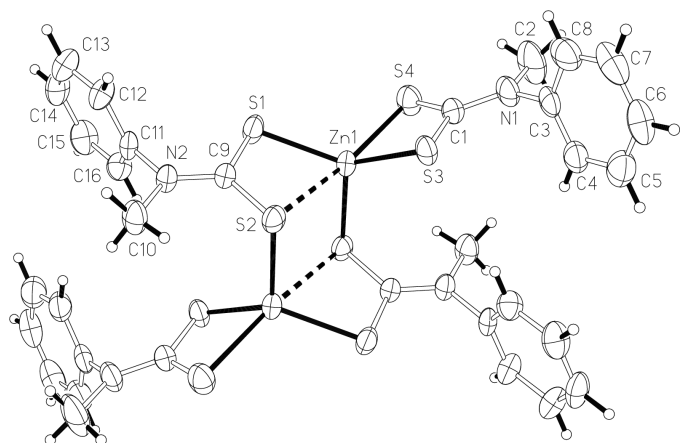


Figure 1
ORTEPII (Johnson, 1976) plot of (I), with ellipsoids at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

Experimental

The title compound, (I), was synthesized from zinc dichloride (10 mmol), methylaniline (20 mmol) and carbon disulfide (20 mmol) in ethanol solution, according to the procedure described for the synthesis of such compounds (Baba *et al.*, 2001a,b). Crystals were obtained by the use of a dichloromethane–methanol (1/1) mixture. Elemental analysis, found (calculated): C 43.69 (44.70), H 3.75 (3.75), N 6.52 (7.52), S 29.82% (29.83%).

Crystal data

$[\text{Zn}_2(\text{C}_8\text{H}_8\text{NS}_2)_4]$
 $M_r = 859.84$
 Monoclinic, $P2_1/c$
 $a = 12.7276$ (1) Å
 $b = 6.6693$ (1) Å
 $c = 22.2508$ (1) Å
 $\beta = 100.669$ (1)°
 $V = 1856.09$ (3) Å³
 $Z = 2$

$D_x = 1.538$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 8192 reflections
 $\theta = 1.6$ – 28.2 °
 $\mu = 1.77$ mm⁻¹
 $T = 298$ (2) K
 Block, colorless
 $0.46 \times 0.22 \times 0.20$ mm

Data collection

Bruker CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.496$, $T_{\max} = 0.718$
 12082 measured reflections

4460 independent reflections
 3383 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.089$
 $\theta_{\text{max}} = 28.2$ °
 $h = -16 \rightarrow 15$
 $k = -8 \rightarrow 8$
 $l = -29 \rightarrow 24$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.114$
 $S = 0.95$
 4460 reflections
 210 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0385P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.56$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.12$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Zn1–S1	2.316 (1)	Zn1–S3	2.348 (1)
Zn1–S2	2.980 (1)	Zn1–S4	2.459 (1)
Zn1–S2 ⁱ	2.378 (1)		
S1–Zn1–S2 ⁱ	105.9 (1)	S3–Zn1–S4	76.1 (1)
S1–Zn1–S3	130.9 (1)	C9–S1–Zn1	96.8 (1)
S1–Zn1–S4	112.2 (1)	C9–S2–Zn1 ⁱ	99.9 (1)
S2 ⁱ –Zn1–S3	117.7 (1)	C1–S3–Zn1	83.8 (1)
S2 ⁱ –Zn1–S4	107.7 (1)	C1–S4–Zn1	80.8 (1)

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

The H atoms were positioned geometrically and allowed to ride on their parent C atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for the methylene H atoms and $1.5U_{\text{eq}}(\text{C})$ for the methyl H atoms.

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXL97.

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