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Bis(μ-*N*-ethyl-*N*-isopropyldithiocarbamato-*S*:*S*′)bis-[(*N*-ethyl-*N*-isopropyldithiocarbamato-*S*,*S*′)zinc(II)]

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.038
wR factor = 0.094
Data-to-parameter ratio = 16.5

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

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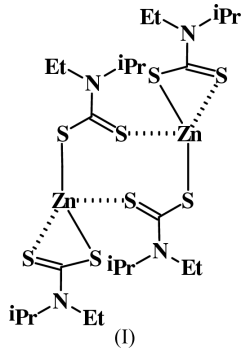
In the centrosymmetric title compound, $[Zn_2(C_6H_{12}NS_2)_4]$, one dithiocarbamate group chelates the Zn atom, whereas the other is bonded to two Zn atoms.

Comment

Zinc(II) dithiocarbamates adopt centrosymmetric dimeric structures (Cox & Tiekink, 1997). The geometry of the Zn atom in the title compound, (I), is similar to that found in the butylethyldithiocarbamate (Baba *et al.*, 2001) where the intra-dimer interaction is shorter and the bridging distance is longer.



(I)

Experimental

Carbon disulfide was added to an ethanol solution of ethylisopropyllamine at 277 K followed by an ethanol solution of zinc chloride. The mixture was stirred vigorously and then set aside. The solid that separated was isolated and recrystallized from ethanol to afford the title compound.

Crystal data

$[Zn_2(C_6H_{12}NS_2)_4]$
M_r = 779.88
Monoclinic, $P2_1/n$
a = 10.8646 (1) Å
b = 15.0517 (1) Å
c = 11.2934 (1) Å
β = 101.419 (1)°
V = 1810.26 (3) Å^3
Z = 2
D_x = 1.431 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8192 reflections
θ = 2.3–28.3°
μ = 1.81 mm^{-1}
T = 298 (2) K
Block, colorless
0.48 × 0.44 × 0.30 mm

Data collection

Siemens CCD area-detector diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
T_{min} = 0.477, T_{max} = 0.613
12 713 measured reflections
4432 independent reflections
3629 reflections with $(I) > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 28.3°
$h = -7 \rightarrow 14$
$k = -19 \rightarrow 20$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0463P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.038$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.094$	$\Delta\rho_{max} = 0.68$ e Å^{-3}
$S = 0.97$	$\Delta\rho_{min} = -0.62$ e Å^{-3}
4432 reflections	Extinction correction: *SHELXL*97
269 parameters	Extinction coefficient: 0.033 (1)
All H-atom parameters refined	

Table 1
Selected geometric parameters (Å, °).

Zn1—S1	2.357 (1)	Zn1—S4	2.707 (1)
Zn1—S2	2.460 (1)	Zn1—S4^{i}	2.408 (1)
Zn1—S3	2.362 (1)		
S1—Zn1—S2	75.1 (1)	S2—Zn1—S4^{i}	103.8 (1)
S1—Zn1—S3	139.7 (1)	S3—Zn1—S4	70.9 (1)
S1—Zn1—S4	92.6 (1)	S3—Zn1—S4^{i}	102.9 (1)
S1—Zn1—S4^{i}	114.9 (1)	S4—Zn1—S4^{i}	93.3 (1)
S2—Zn1—S3	110.0 (1)	Zn1^{i}—S4—Zn1	86.7 (1)
S2—Zn1—S4	161.9 (1)		

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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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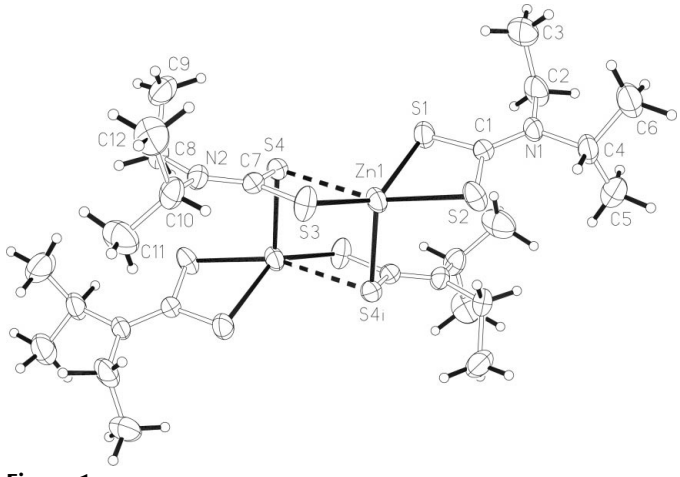

Figure 1
*ORTEP*II (Johnson, 1976) plot of the title compound at the 50% probability level. H atoms are shown as circles of arbitrary radii.

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