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Crystallographic report

Bis(*N*,*N*-dibenzyldithiocarbamato)zinc(II)

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The structure of $Zn[S_2CN(CH_2Ph)_2]_2$ features, in contrast to many related analogues, a mononuclear species with two chelating dithiocarbamate ligands that form a distorted tetrahedral array around the zinc centre; the molecule has two-fold symmetry. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; zinc; dithiocarbamate

COMMENT

The molecular structure of $Zn[S_2CN(CH_2Ph)_2]_2$, Fig. 1, features a pair of chelating dithiocarbamate ligands, each of which forms significantly different Zn–S bond lengths; the two ligands are related via a two-fold axis. The coordination geometry around the zinc atom is best described as a very highly distorted tetrahedral arrangement of the four sulfur atoms. This complex represents a rare example of a monomeric structure within the zinc-triad of 1,1′-dithiolates.[1] Thus, the overall solid-state structure is similar to the only other known examples of monomeric binary zinc dithiocarbamates, viz. bis[*N*,*N*-dicylohexyldithiocarbamato]zinc(II)[2] and bis[*N*-*n*-butyl-*N*-(3,5-di-*tert*-butyl-2-hydroxybenzyl)dithiocarbamato]zinc(II).[3] The title compound is isomorphous with the mercury analogue.[4]

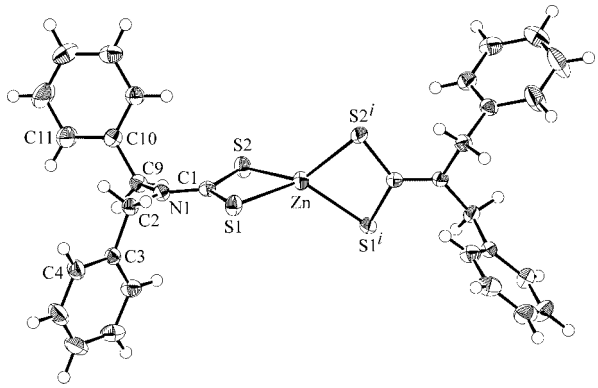

Figure 1. Molecular structure of $Zn[S_2CN(CH_2Ph)_2]_2$. Key geometric parameters: Zn–S1 2.3629(3), Zn–S2 2.3312(3), N1–C1 1.3308(16) Å. S1–Zn–S2 78.043(11), S1–Zn–S1^i 126.243(19), S1–Zn–S2^i 123.975(12), S2–Zn–S2^i 134.23(2)°. Symmetry code *i*: $-x$, y, $3/2 - z$.

EXPERIMENTAL

$Zn[S_2CN(CH_2Ph)_2]_2$ was obtained commercially (BDH); m.p. 178–179 °C. IR (KBr): ν(C–S) 984 and ν(C–N) 1485 cm^{-1}. ^{1}H NMR (300.13 MHz, $CDCl_3$): $\delta = 5.08$ [s, 8H, CH_2], 7.50–7.28 ppm [complex pattern, 20H, phenyl]; ^{13}C NMR: $\delta = 206.1$ [C_{quat}], 134.4 [C_{ipso}], 128.9 [C_{ortho}], 128.2 [C_{meta}], 128.0 [C_{para}], 55.7 ppm [CH_2]. Colourless crystals of this material were grown by solvent evaporation from a dichloromethane solution layered with diethyl ether at 22 °C. Data were collected at 198(1) K on a Bruker AXS P4/SMART 1000 diffractometer for a parallelepiped crystal of dimensions 0.20 × 0.23 × 0.50 mm^3. $C_{30}H_{28}N_2S_4Zn$, $M = 610.15$, orthorhombic, *Pbcn*, $a = 16.0968(7)$, $b = 18.9388(8)$, $c = 9.2825(4)$ Å, $V = 2829.8(2)$ Å^3, $Z = 4$, 3220 unique data (θ_{max} 27.5°), 2929 data with $I \geq 2\sigma(I)$, R 0.023 = (obs. data), wR 0.063 = (all data). Programs

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