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Crystallographic report

Bis[bis(*N*,*N*-dibenzyldithiocarbamato)zinc(II)](4,4′-bipyridine)

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The centrosymmetric structure of {Zn[$S_2CN(CH_2Ph)_2$]$_2$}$_2$(4,4′-bipy) features chelating dithiocarbamate ligands so that a trigonal bipyramidal NS_4 coordination geometry for zinc results. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; zinc; dithiocarbamate; diimine; adduct

COMMENT

The centrosymmetric dinuclear structure of {Zn[$S_2CN(CH_2Ph)_2$]$_2$}$_2$(4,4′-bipy), Fig. 1, features two chelating dithiocarbamate ligands, each of which forms disparate Zn–S bonds. The zinc atoms are bridged by a 4,4′-bipyridine ligand so that a five-coordinate NS_4 geometry results that is best described as trigonal bipyramidal in which the axial positions are defined by the more weakly coordinated S2 and S4 atoms. The overall structure is similar, for example, to those reported for {Zn[$S_2CN(^iPr)_2$]$_2$}$_2$(4,4′-bipy)[1] and {Zn[S_2CNEt_2]$_2$}$_2$(4,4′-bipy).[2,3]

EXPERIMENTAL

A solution of 4,4′-bipyridine (1 mmol) in tetrahydrofuran (THF; 10 ml) was added to a solution of zinc dibenzyldithiocarbamate (1 mmol), prepared by standard methods, in THF (20 ml). The mixture was stirred for 2 h at room temperature and filtered to give a pale yellow solution. Yellow crystals were obtained from the slow evaporation of the THF solution of the compound; m.p. 485–486 K. IR (KBr): ν(C–S) 991 and ν(C–N) 1451, 1492 cm^{-1}. ^{1}H

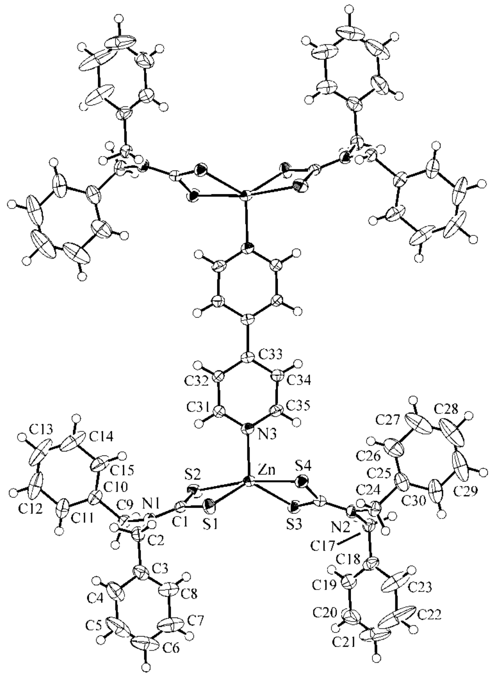

Figure 1. Molecular structure of {Zn[$S_2CN(CH_2Ph)_2$]$_2$}$_2$(4,4′-bipy); the mid-point of the C33–C33^i bond lies on a centre of inversion. Key geometric parameters: Zn–S1 2.3183(6), Zn–S2 2.5982(6), Zn–S3 2.3294(6), Zn–S4 2.6122(6), Zn–N3 2.0552(16) Å; S1–Zn–S2 73.089(18), S1–Zn–S3 128.34(2), S1–Zn–S4 99.16(2), S1–Zn–N3 115.45(5), S2–Zn–S3 106.73(2), S2–Zn–S4 170.131(19), S2–Zn–N3 95.72(5), S3–Zn–S4 72.975(18), S3–Zn–N3 115.91(5), S4–Zn–N3 93.15(5)°. Symmetry code *i*: $1-x$, $-y$, $1-z$.

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NMR (300.13 MHz, $CDCl_3$): $\delta = 5.12$ [s, CH_2], 7.26–7.40 [complex pattern, phenyl], 7.70–7.72 [m, C*H*CHN], 9.07–9.09 ppm [m, C*H*N]. Intensity data were collected at 223 K on a Bruker AXS SMART CCD for a yellow block $0.13 \times 0.44 \times 0.44$ mm^3. $C_{70}H_{64}N_6S_8Zn_2$, $M =$ 1376.50, triclinic, $P\overline{1}$, $a = 10.6878(7)$, $b = 12.6278(8)$, $c = 13.2586(8)$ Å, $\alpha = 93.090(1)$, $\beta = 104.488(1)$, $\gamma = 108.270(1)°$, $V = 1628.05(18)$ Å^3, $Z = 1$ (dimer), 9343 unique data (θ_{max} 30.1°), 7440 data with $I \geq 2\sigma(I)$, $R = 0.046$ (obs. data), $wR = 0.119$ (all data). Disorder in the phenyl groups could not be resolved satisfactorily. Programs used: teXsan, DIRDIF, SHELXL-97 and ORTEP. CCDC deposition number: 215779.

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