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Crystallographic report

Bis[bis(*N*,*N*-diethyldithiocarbamato)zinc(II)] (*trans*-1,2-bis(4-pyridyl)ethylene)*trans*-1,2-bis(4-pyridyl)ethylene lattice adduct

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The dimeric and centrosymmetric structure of [$Zn(S_2CNEt_2)_2$(*trans*-$NC_5H_4C(H){=}C(H)C_5H_4N$)]$_2$ shows bidentate coordination by the dithiocarbamate ligands and a distorted square pyramidal geometry for zinc, defined by a NS_4 donor set with the N atom in the apical position. The compound co-crystallises with a centrosymmetric molecule of *trans*-$NC_5H_4C(H){=}C(H)C_5H_4N$ that does not form a significant interaction to the Zn atom. Copyright © 2003 John Wiley & Sons, Ltd.

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

COMMENT

Dimeric, e.g. [$Zn(S_2CN^iPr_2)_2]_2$(4,4′-bipy),[1] and polymeric, e.g. [$Zn(S_2CO^iPr)_2$(4,4′-bipy)]$_\infty$,[2] *trans*-diimine adducts of zinc dithiocarbamates are known and can be prepared simply by altering the Zn : diimine ratio. Crystals of the title compound were obtained from a solution containing $Zn(S_2CNEt_2)_2$ and *trans*-$NC_5H_4C(H){=}C(H)C_5H_4N$ in the ratio 1 : 1. Rather than isolating the expected polymeric structure, X-ray structure determination revealed the formation of a centrosymmetric and dimeric structure (Fig. 1) and the inclusion of a non-coordinating and centrosymmetric *trans*-$NC_5H_4C(H){=}C(H)C_5H_4N$ molecule in the lattice. In the complex, the dithiocarbamate ligands are chelating and the coordination geometry is best described as being square pyramidal with the nitrogen atom occupying the axial position.

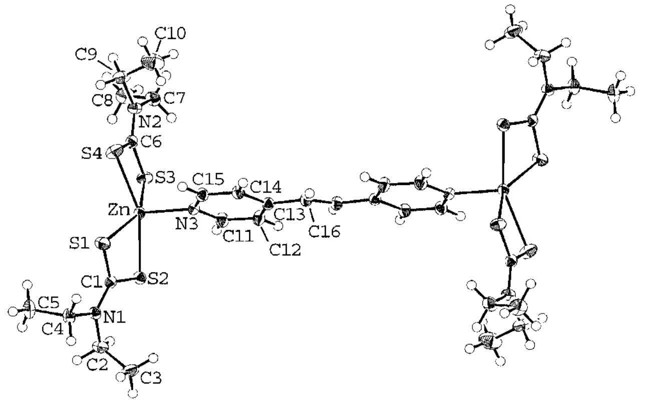

Figure 1. Dimeric structure of [$Zn(S_2CNEt_2)_2]_2$(*trans*-$NC_5H_4C(H){=}C(H)C_5H_4N$); the co-crystallized *trans*-$NC_5H_4C(H){=}C(H)C_5H_4N$ molecule is not shown for reasons of clarity. Key geometric parameters: Zn–S(1) 2.4169(8), Zn–S(2) 2.4770(8), Zn–S(3) 2.4099(8), Zn–S(4) 2.4914(9), Zn–N(3) 2.077(2), S(1)–C(1) 1.730(3), S(2)–C(1) 1.721(3), S(3)–C(6) 1.727(3), S(4)–C(6) 1.715(3), C(1)–N(1) 1.319(4), C(6)–N(2) 1.325(4) Å; S(1)–Zn–S(2) 73.84(3), S(1)–Zn–S(3) 151.01(3), S(1)–Zn–S(4) 94.78(3), S(1)–Zn–N(3) 108.17(7), S(2)–Zn–S(3) 107.51(3), S(2)–Zn–S(4) 158.76(3), S(2)–Zn–N(3) 99.18(7), S(3)–Zn–S(4) 73.76(3), S(3)–Zn–N(3) 100.27(7), S(4)–Zn–N(3) 101.44(7)°.

EXPERIMENTAL

Bright-yellow crystals were isolated from a 0.5/1 acetonitrile/chloroform solution containing equimolar amounts of $Zn(S_2CNEt_2)_2$[3] and *trans*-$NC_5H_4C(H){=}C(H)C_5H_4N$ (Aldrich); m.p. 197–198 °C. IR (KBr): ν(C–S) 996 and ν(C–N) 1426 and 1491 cm^{-1}. Intensity data were collected at 183 K on a Bruker AXS SMART CCD diffractometer for a yellow plate 0.06 × 0.11 × 0.21 mm^3. $C_{22}H_{30}N_4S_4Zn$, $M =$

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544.11, triclinic, $P\overline{1}$, $a = 9.5311(10)$, $b = 12.2820(14)$, $c = 12.9165(10)$ Å, $\alpha = 63.369(2)$, $\beta = 80.547(3)$, $\gamma = 68.465(2)^\circ$, $V = 1257.3(2)$ Å^3, $Z = 2$, 7196 unique data ($\theta_{\max}$ 30.0°), $R = 0.073$ (all data), $wR = 0.126$ (all data), $\rho_{\max} = 2.16$ e$^-$ Å^{-3} (near zinc). Programs used: teXsan, DIRDIF, SHELXL, and ORTEP. CCDC deposition number: 200067.

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