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Crystallographic report

(2,9-Dimethyl-1,10-phenanthroline)bis-(*N*,*N*-pyrrolidinedithiocarbamato)zinc(II) chloroform hemihydrate

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The mononuclear structure of $Zn(S_2C(N(CH_2)_2)_4)_2$(2,9-Me_2-1,10-phen) shows monodentate coordination by the dithiocarbamate ligands and a distorted tetrahedral geometry for zinc, defined by an N_2S_2 donor set, results. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; zinc; dithiocarbamate; diimine adduct

COMMENT

Diimine adducts of zinc dithiocarbamates, including pyrrolidinedithiocarbamate, normally exhibit six-coordination and a distorted octahedral environment (e.g. see Refs 1–3). By contrast, in the title compound, which features the sterically hindered diimine, 2,9-dimethyl-1,10-phenanthroline, the dithiocarbamate ligands are monodentate, so that a distorted tetrahedral geometry results (Fig. 1). In the analogous cadmium structure, chelating ligands are found, leading to a distorted octahedral structure.[4] The compound crystallizes as a chloroform and hemi-aquo solvate.

EXPERIMENTAL

Pale-yellow crystals were isolated from a 0.5/1 acetonitrile/chloroform solution containing equimolar amounts of $Zn(S_2C(N(CH_2)_2)_4)_2$[2] and 2,9-Me_2phen (Aldrich); m.p. 236–237 °C. IR (KBr): ν(C–S) 1006 and ν(C–N) 1403 cm^{-1}. Intensity data were collected at 183 K on a Bruker AXS SMART CCD diffractometer for a yellow block 0.09 × 0.10 × 0.34 mm^3. $C_{25}H_{30}Cl_3N_4O_{0.5}S_4Zn$, M = 694.49, triclinic, $P\overline{1}$, a = 10.0706(8), b = 10.7260(9), c = 14.0947(12) Å, α = 83.526(2), β = 89.515(2), γ = 89.855(2)°, V = 1512.7(2) $Å^3$, Z = 2, 8654 unique data (θ_{max}30.1°), R = 0.099 (all data), wR = 0.197 (all data), ρ_{max} = 1.28 e^- $Å^{-3}$ (near Cl3). Programs used: teXsan, DIRDIF, SHELXL, and ORTEP. CCDC deposition number: 200065.

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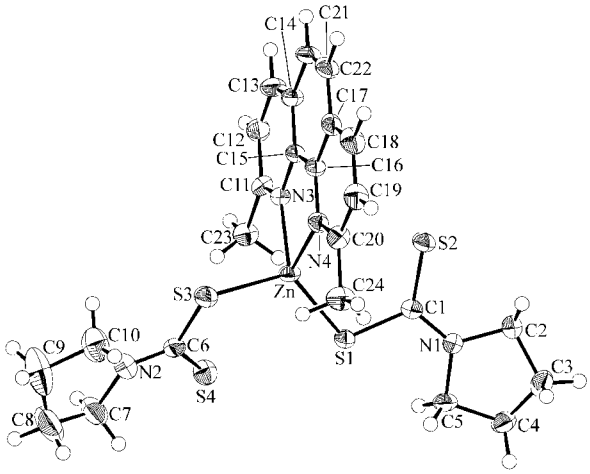

Figure 1. Molecular structure of $Zn(S_2C(N(CH_2)_2)_4)_2$(2,9-Me_2-1,10-phen); solvent molecules have been omitted for reasons of clarity. Key geometric parameters: Zn–S(1) 2.2701(11), Zn···S(2) 3.3380(12), Zn–S(3) 2.3193(12), Zn···S(4) 3.3992(12), Cd–N(3) 2.069(3), Cd–N(4) 2.084(3), S(1)–C(1) 1.759(4), S(2)–C(1) 1.680(4), S(3)–C(6) 1.738(4), S(4)–C(6) 1.695(4), C(1)–N(1) 1.332(5), C(6)–N(2) 1.313(5) Å; S(1)–Cd–S(3) 121.81(4), S(1)–Cd–N(3) 118.69(10), S(1)–Cd–N(4) 122.67(9), S(3)–Cd–N(3) 108.64(9), S(3)–Cd–N(4) 95.32(10), N(3)–Zn–N(4) 81.00(12)°.

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