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Crystallographic report

Bis(*N,N*-diethyldithiocarbamato)(2,9-dimethyl-1,10-phenanthroline)cadmium(II)

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The mononuclear structure of $Cd(S_2CNEt_2)_2$(2,9-Me_2-1,10-phenanthroline) shows symmetric coordination of the dithiocarbamate ligands and a distorted octahedral geometry for cadmium, defined by an N_2S_4 donor set, results. Copyright © 2002 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; cadmium; dithiocarbamate; diimine adduct

COMMENT

Mononuclear[1–3] and binuclear[4,5] Lewis base adducts are known for the cadmium bis(dithiocarbamates) for which coordination geometries vary from octahedral[1,2] to trigonal prismatic[3] for diimine adducts, and trigonal bipyramidal[4] to square pyramidal[5] for phosphine adducts. In the present structure (Fig. 1), $Cd(S_2CNEt_2)_2$(2,9-Me_2-1,10-phen), which has crystallographic two fold symmetry, by virtue of the presence of chelating dithiocarbamate ligands, the cadmium centre exists in a distorted octahedral environment defined by an N_2S_4 donor set as has been found previously in the related 2,2′-bipyridine[1] and 1,10-phenanthroline[2] adducts.

EXPERIMENTAL

Pale-yellow crystals were isolated from an acetonitrile/chloroform (0.5:1) solution containing equimolar amounts of $Cd(S_2CNEt_2)_2$ and 2,9-Me_2-phen (Aldrich); m.p. 259–262 °C. IR (KBr, cm^{-1}): ν(C—S) 991 and ν(C—N) 1416. Intensity data were collected at 183 K on a Bruker AXS SMART CCD diffractometer for a yellow block 0.07 × 0.13 × 0.39 mm^3. $C_{24}H_{32}CdN_4S_4$, M = 617.2, monoclinic, $P2_1/n$, a = 11.0884(7), b = 9.9570(6), c = 25.0055(15) Å, β = 93.067(1)°, V = 2756.8(3) $Å^3$, Z = 4, 8015 unique data (θ_{max} 30.0°), R = 0.065 (all data), wR = 0.107 (all data), ρ_{max} = 1.29 e^- $Å^{-3}$ (near Cd). Programs used: teXsan, DIRDIF, SHELXL, and ORTEP. CCDC deposition number: 193903.

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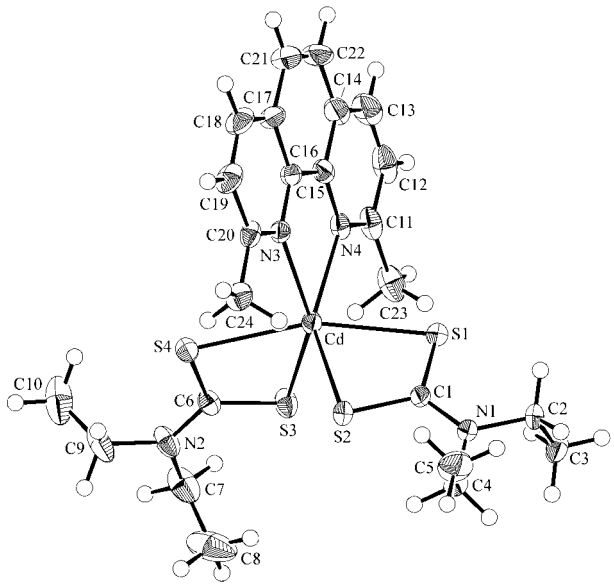

Figure 1. Molecular structure of $Cd(S_2CNEt_2)_2$(2,9-Me_2-1,10-phenanthroline). Key geometric parameters: Cd—S(1) 2.6735(8), Cd—S(2) 2.6818(8), Cd—S(3) 2.6807(8), Cd—S(4) 2.7063(8), Cd—N(3) 2.401(2), Cd—N(4) 2.436(2), S(1)—C(1) 1.725(3), S(2)—C(1) 1.712(3), S(3)—C(6) 1.711(3), S(4)—C(6) 1.720(3), C(1)—N(1) 1.334(4), C(6)—N(2) 1.336(4) Å; S(1)—Cd—S(2) 67.22(2), S(1)—Cd—S(3) 103.24(3), S(1)—Cd—S(4) 162.18(2), S(1)—Cd—N(3) 106.55(6), S(1)—Cd—N(4) 83.86(6), S(2)—Cd—S(3) 95.16(3), S(2)—Cd—S(4) 98.18(2), S(2)—Cd—N(3) 106.58(6), S(2)—Cd—N(4) 149.06(6), S(3)—Cd—S(4) 66.70(2), S(3)—Cd—N(3) 148.11(6), S(3)—Cd—N(4) 102.23(6), S(4)—Cd—N(3) 86.96(6), S(4)—Cd—N(4) 112.12(6), N(3)—Cd—N(4) 70.32(8)°.

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