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Crystallographic report

Bis[bis(*N*,*N*-dibenzyldithiocarbamato)cadmium(II)]

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The centrosymmetric structure of $\{Cd[S_2CN(CH_2Ph)_2]_2\}_2$ features both bridging and chelating dithiocarbamate ligands so that a square pyramidal S_5 coordination geometry results. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; cadmium; dithiocarbamate

COMMENT

The centrosymmetric dinuclear structure of $\{Cd[S_2CN(CH_2Ph)_2]_2\}_2$, Fig. 1, features two tridentate dithiocarbamate ligands that μ_2-bridge via one sulfur atom each to two cadmium atoms leading to the formation of a Cd_2S_2 core; the other ligands are chelating. This arrangement leads to five-coordinate cadmium centres that are best described as existing in square pyramidal geometries. The overall structure conforms to the predominant motif found for the other binary cadmium dithiocarbamates that have been characterized crystallographically;[1] the exception is that of $[Cd(S_2CNnBu_2)_2]_2$, which has two fold symmetry, so that the chelating dithiocarbamate ligands lie to one side of the molecule.[2]

EXPERIMENTAL AND RESULTS

A solution of $CdCl_2$ (0.5 mmol) in water (10 ml) was added to a solution of sodium dibenzyldithiocarbamate (1 mmol), prepared by standard methods, in ethanol (20 ml). The mixture was stirred for 2 h at room temperature and the precipitated compound was filtered off, washed with ethanol then with diethyl ether and dried in

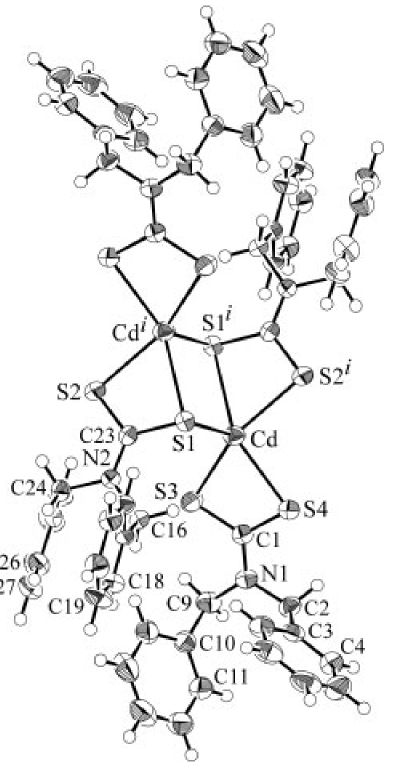

Figure 1. Molecular structure of $\{Cd[S_2CN(CH_2Ph)_2]_2\}_2$. Key geometric parameters: Cd–S1 2.6200(6), Cd–S1^i 2.7875(7), Cd–S2^i 2.5834(7), Cd–S3 2.5491(7), Cd–S4 2.6030(7) Å; S1–Cd–S1^i 92.461(19), S1–Cd–S2^i 101.17(2), S1–Cd–S3 106.64(2), S1–Cd–S4 118.20(2), S1^i–Cd–S2^i 67.060(19), S1^i–Cd–S3 112.60(2), S1^i–Cd–S4 147.53(2), S2^i–Cd–S3 152.15(2), S2^i–Cd–S4 94.88(2), S3–Cd–S4 70.70(2)°. Symmetry operation *i*: $-1-x$, $-y$, $1-z$.

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vacuum. Colourless crystals were obtained from the slow evaporation of an acetonitrile solution of the compound; m.p. 195 °C. IR (KBr): ν(C–S) 972 and ν(C–N) 1454, 1480, 1495 cm^{-1}. ^1H NMR (300.13 MHz, $CDCl_3$): $\delta = 5.16$ [s, 2H, CH_2], 7.21–7.46 ppm [complex pattern, 5H, aromatic]. Intensity data were collected at 223 K on a Bruker AXS SMART CCD for a colourless block $0.15 \times 0.34 \times 0.34$ mm^3. $C_{30}H_{28}CdN_2S_4$, $M = 657.2$, monoclinic, $P2_1/n$, $a = 11.1098(4)$, $b = 15.6325(5)$, $c = 16.6695(6)$ Å, $\beta = 97.9220(10)°$, $V = 2867.43(17)$ $Å^3$, $Z = 4$, 8313 unique data (θ_{max} 30.0°), 6404 data with $I \geq 2\sigma(I)$, $R = 0.044$ (obs. data), $wR = 0.099$ (all data). Programs used: teXsan, DIRDIF, SHELXL-97 and ORTEP. CCDC deposition number: 213433.

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