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Crystallographic report

A new polymorph for bis[bis(*N*,*N*-dibenzyldithiocarbamato)cadmium(II)]

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The title compound is a centrosymmetric dimer with each cadmium in a distorted CdS_5 square pyramidal geometry. The Cd–S bond distances range from 2.5626(11) to 2.8459(11) Å.

KEYWORDS: cadmium; dithiocarbamate; crystal structure

COMMENT

The main-group elements zinc, cadmium and mercury readily form dithiocarbamate complexes.[1] Two independent and centrosymmetric molecules comprise the asymmetric unit in the title compound, $[Cd(dbzdtc)_2]_2$; one molecule is shown in Fig. 1. The cadmium atom is in a distorted square pyramidal coordination environment with Cd–S bonds in the range 2.5626(11) to 2.8459(11) Å; as a consequence, the C–S bonds are asymmetric. The mean thioureide bond distance is 1.344(4) Å. The crystal structure of a monoclinic polymorph of $[Cd(dbzdtc)_2]_2$ has been reported recently.[2]

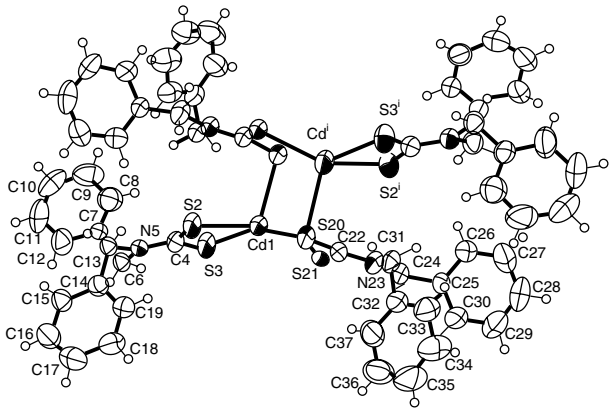

Figure 1. Selected bond lengths (Å) and bond angles (°) for one of the independent molecules of $[Cd(dbzdtc)_2]_2$: Cd1–S2 2.5834(11), Cd–S20 2.6467(11), Cd1–S21 2.5626(11), Cd1–S3 2.6158(11), Cd–S20 2.8459(11), S2–C4 1.733(3), S3–C4 1.720(3), C4–N5 1.345(4), S20–C22 1.747(3), S21–C22 1.719(3), C22–N23 1.337(4); S2–Cd1–S21 150.94(3), S3–Cd1–S21 114.69(4), S2–Cd1–S3 69.68(3), S20^{i}–Cd1–S21 99.39(3), S21–Cd1–S20 66.72(3), S20–Cd1–S20^{i} 93.42(3). Symmetry operation, i: $-x$, $-y$, $-z$.

EXPERIMENTAL

Dibenzylamine (10 mmol, 2.0 ml) in ethanol (10 ml) and carbon disulfide (10 mmol, 0.6 ml) in ethanol (10 ml) under cold condition (5 °C) were mixed thoroughly and stirred. The resulting yellow dithiocarbamic acid was mixed with $Cd(NO_3)_2$ (5 mmol, 1.5 g) in water (5 ml) with constant stirring. The precipitated complex was filtered, washed with water, alcohol and was then dried in air. Anal. Found: C, 53.9; H, 4.0; N, 3.9. Calc. for the complex: C, 54.9; H, 4.2; N, 4.2%. Electronic spectrum: CT band at 280 nm. Thioureide band at 1527 cm^{-1}(IR). Suitable single crystals were obtained from benzene solution. The intensity data were collected on a Bruker AXS SMART CCD diffractometer with a colourless crystal $0.19 \times 0.26 \times 0.39$ mm^3. $C_{60}H_{56}N_4S_8Cd_2$, $M = 1314.37$, triclinic, $P\bar{1}$, $a = 10.226(2)$ $b = 16.545(3)$, $c = 17.882(2)$Å, $\alpha = 81.36(2)$, $\beta = 80.45(2)$, $\gamma = 85.66(2)°$, $V = 2945.7(9)$Å^3, $Z = 2$, 8105 unique reflections ($\theta_{max} = 28.1°$). $R = 0.037$, $R_w = 0.085$, $\rho = 1.48$ e^- Å^{-3}. Programs used: SHELXTL-NTV5.1. CCDC deposition number: 209 678.

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