APPLIED ORGANOMETALLIC CHEMISTRY
Appl. Organometal. Chem. 2004; **18**: 104
Main Group Metal Compounds
Published online in Wiley InterScience (www.interscience.wiley.com). DOI:10.1002/aoc.582

Crystallographic report

Bis(*N*,*N*-dibenzyldithiocarbamato)mercury(II)

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Received 7 November 2003; Revised 8 November 2003; Accepted 9 November 2003

The monomeric structure of $Hg[S_2CN(CH_2Ph)_2]_2$, in which the mercury atom lies on a two fold axis that relates the unsymmetrically chelating dithiocarbamate ligands, features a severely distorted tetrahedral geometry. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; mercury; dithiocarbamate

COMMENT

The mercury atom in $Hg[S_2CN(CH_2Ph)_2]_2$, Fig. 1, lies on a two fold axis and exists in a grossly distorted tetrahedral geometry as the result of two unsymmetrically coordinating dithiocarbamate ligands. This structure, along with the isomorphous zinc analogue,[1] is consistent with 'steric control over molecular aggregation' for zinc-triad 1,1-dithiolate structures.[2] As such, the mercury (and zinc[1]) structure is a member of the least common, i.e. monomeric, motif owing to the steric bulk of the N-bound groups. In this context, it is interesting that the dimeric cadmium analogue[3] is consistent with known structures owing to its uncluttered dimeric motif.[2]

Experimental and Results

Colourless crystals, prepared by standard methods,[4] were obtained from the slow evaporation of a chloroform solution of the compound; m.p. 209–210 °C. IR (KBr): ν(C–S) 999 and ν(C–N) 1474 cm^{-1}. ^1H NMR ($CDCl_3$): $\delta = 5.02$ [s, 2H, CH_2], 7.34–7.43 ppm [complex pattern, 5H, aromatic]. ^{13}C NMR: $\delta = 206.8$ [C_{quat}], 134.5 [C_{ipso}], 129.3 [C_{ortho}], 128.2 [C_{meta}], 127.4 [C_{para}], 58.1 ppm [CH_2]. Intensity data were collected at 223 K on a Bruker AXS SMART CCD for a colourless plate $0.05 \times 0.16 \times 0.31$ mm^3. $C_{30}H_{28}HgN_2S_4$, $M = 745.37$, orthorhombic, *Pbcn*, $a = 16.3851(5)$, $b = 18.5774(6)$, $c = 9.3190(3)$ Å, $V = 2836.63(16)$ $Å^3$, $Z = 4$, 4124 unique data (θ_{max} 30.0°), 3271 data with $I \geq 2\sigma(I)$, R 0.050 = (obs. data), wR 0.103 = (all data); $\rho_{max} = 2.13$ e^- $Å^{-3}$ (near mercury). Programs used: teXsan, DIRDIF, SHELXL-97 and ORTEP. CCDC deposition number: 223843.

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Contract/grant sponsor: National University of Singapore; Contract/grant number: R-143-000-213-112.

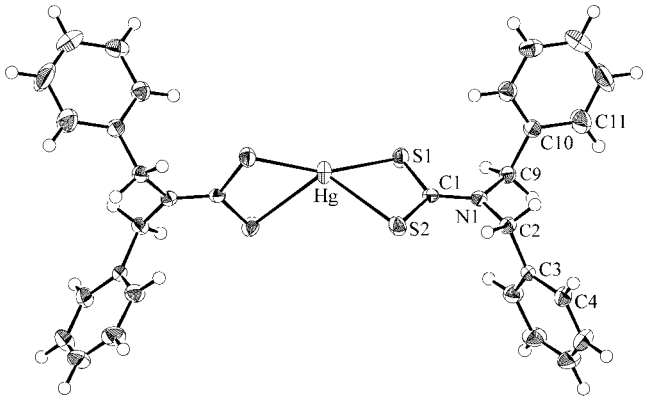

Figure 1. Molecular structure of $Hg[S_2CN(CH_2Ph)_2]_2$. Key geometric parameters: Hg–S1 2.3968(12), Hg–S2 2.7896(12), C1–S1 1.753(4), C1–S2 1.703(4) Å; S1–Cd–S2 69.69(4), S1–Cd–$S1^i$ 160.34(6), S1–Cd–$S2^i$ 121.90(4), S2–Cd–$S2^i$ 115.86(5)°. Symmetry operation i: $-x$, y, $1/2 - z$.

Acknowledgements

The National University of Singapore (R-143-000-213-112) is thanked for support.

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