APPLIED ORGANOMETALLIC CHEMISTRY
Appl. Organometal. Chem. 2003; **17**: 194
Main Group Metal Compounds AOC
Published online in Wiley InterScience (www.interscience.wiley.com). DOI:10.1002/aoc.395

Crystallographic report

Phenyl(*N*,*N*-di-*n*-propyldithiocarbamato)mercury(II)

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Received 1 October 2002; Revised 7 October 2002; Accepted 8 October 2002

The structure of $PhHg(S_2CNPr_2)$ shows a distorted linear geometry about mercury defined by a sulfur and a carbon atom. Centrosymmetric molecules aggregate via Hg···S interactions to form loosely associated dimers. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; mercury; dithiocarbamate; organometallic

COMMENT

The different types of molecular aggregation in the organomercury 1,1-thiolate structures have been highlighted recently.[1] In this way, facilitated by Hg···S interactions, loosely associated dimers, polymeric chains and tapes have been delineated,[1,2] and it is in this connection that the title compound, $PhHg(S_2CNPr_2)$, was investigated. To a first approximation, the mercury atom exists in a C—Hg—S linear geometry. Considerable distortion from the ideal 180° angle may be traced to the presence of close intra- and intermolecular Hg···S interactions that lead to a chair-like structure comprising two mononuclear units, as shown in Figure 1. Such aggregation is normally adopted by organomercury dithiocarbamate structures.[1–4]

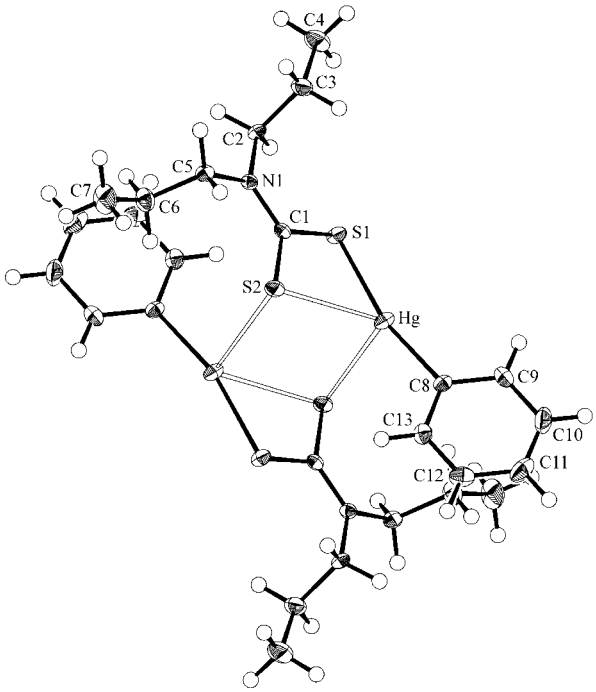

Figure 1. Molecular structure of $PhHg(S_2CNPr_2)_2$. Key geometric parameters: Hg—S(1) 2.4033(9), Hg···S(2) 2.9093(10), Hg···S(2)^i 3.1809(10), Hg—C(8) 2.076(4), S(1)—C(1) 1.752(4), S(2)—C(1) 1.701(4), C(1)—N(1) 1.327(5) Å S(1)—Hg—C(8) 166.76(10), S(1)—Hg···S(2) 67.37(3), Hg—S(1)—C(1) 93.76(12)°. Symmetry operation *i*: $-x$, $-y$, $1-z$.

EXPERIMENTAL

To a stirred dichloromethane (30 ml) solution of PhHgCl (0.2 g, 64 mmol, Aldrich) was added a stoichiometric amount of KS_2CNPr_2 dissolved in water (20 ml). After stirring the mixture for 2 h, the organic layer was separated and dried over $MgSO_4$. The crude product was recrystallized as colourless crystals from a CH_2Cl_2/methanol (1:1) solution; m.p. 56–58 °C. IR (KBr, cm^{-1}): ν(C—S) 995, 1019 and ν(C—N) 1422, 1491. Intensity data were collected at 183 K on a Bruker AXS SMART CCD diffractometer for a block $0.15 \times 0.23 \times 0.52$ mm^3. $C_{13}H_{19}HgNS_2$, $M = 454.0$, monoclinic, $P2_1/n$, $a = 9.9459(6)$, $b = 13.5069(8)$, $c = 12.1273(7)$ Å, $\beta = 109.732(1)°$, $V = 1533.50(16)$ Å^3, $Z = 4$, 4446 unique data ($\theta_{max} = 30.0°$), $R = 0.038$ (all data), $wR = 0.077$ (all data), $\rho_{max} = 2.27$ e$^-$ Å^{-3} (near mercury). Programs used: teXsan, DIRDIF, SHELXL, and ORTEP. CCDC deposition number: 194522.

Acknowledgements

The National University of Singapore is thanked for support (R-143-000-151-112).

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Contract/grant sponsor: National University of Singapore; Contract/grant number: R-143-000-151-112.

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