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*Crystallographic report*

# Bis(*N*-cyclohexyl,*N*-methyldithiocarbamato)zinc(II)

**Meng Yin Chan, Chian Sing Lai and Edward R. T. Tiekink***

Department of Chemistry, National University of Singapore, Singapore 117543, Singapore

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**The mononuclear structure of $Zn[S_2CN(Me)Cy)]_2$ features a tetrahedral zinc center defined by two chelating dithiocarbamate ligands. Copyright © 2004 John Wiley & Sons, Ltd.**

**KEYWORDS:** crystal structure; zinc; dithiocarbamate

## COMMENT

The molecular structure of $Zn[S_2CN(Me)Cy)]_2$, Fig. 1, features two chelating dithiocarbamate ligands with the range of Zn–S distances being relatively narrow at 2.3107(10) to 2.3869(11) Å. The coordination geometry is distorted tetrahedral, as manifested in the range of S–Zn–S angles of 77.81(3)° to 134.01(4)°, with the more acute angle being associated with the $ZnS_2C$ chelate. This complex represents an example of a monomeric structure for the zinc dithiocarbamates, which are usually dimeric.[1] Supramolecular association leading to a dimer is found in the structure of $[Zn(S_2CNMe)_2]_2$,[2,3] but the presence of bulky substituents, such as cyclohexyl[4] and benzyl,[5] precludes aggregation. Nevertheless, in the present case, molecules of $Zn[S_2CN(Me)Cy)]_2$, are orientated, about a crystallographic two fold axis of symmetry, so as to form a virtual dimer, so that the intermolecular Zn···S interactions are 3.5774(11) Å. This suggests a very clear role of the remote *N*-bound substituent in determining the overall molecular structure.

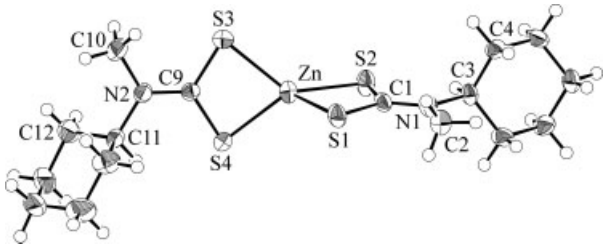


**Figure 1.** Molecular structure of $Zn[S_2CN(Me)Cy)]_2$. Key geometric parameters: Zn–S1 2.3869(11), Zn–S2 2.3107(10), Zn–S3 2.3388(10), Zn–S4 2.3417(10) Å; S1–Zn–S2 77.81(3), S1–Zn–S3 120.47(4), S1–Zn–S4 117.24(4), S2–Zn–S3 133.97(4), S2–Zn–S4 134.01(4), S3–Zn–S4 78.40(3)°.

## EXPERIMENTAL

$Zn[S_2CN(Me)Cy)]_2$ was prepared in 78% yield by standard methods;[4] m.p. 212 °C. IR (KBr): $\nu$(C–S) 970 and $\nu$(C–N) 1481 $cm^{-1}$. Pale-yellow crystals were grown by solvent evaporation of an acetonitrile/chloroform solution (1/3). Data were collected at 223(2) K on a Bruker AXS SMART CCD for a crystal of dimensions $0.10 \times 0.13 \times 0.52$ $mm^3$. $C_{16}H_{28}N_2S_4Zn$, $M = 442.01$, monoclinic, $C2/c$, $a = 16.6990(16)$, $b = 11.1119(11)$, $c = 23.049(2)$ Å, $\beta = 107.114(4)°$, $V = 4087.5(7)$ $Å^3$, $Z = 8$, 5938 unique data ($\theta_{max}$ 30.1°), 4247 data with $I \geq 2\sigma(I)$, $R = 0.073$ (obs. data), $wR = 0.147$ (all data). Programs used: SAINT, SHELXTL, SMART, and SADABS. CCDC deposition number: 230130.

*Correspondence to: Edward R. T. Tiekink, Department of Chemistry, National University of Singapore, Singapore 117543, Singapore.
E-mail: chmtert@nus.edu.sg
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