APPLIED ORGANOMETALLIC CHEMISTRY
Appl. Organometal. Chem. 2005; **19**: 401
Main Group Metal Compounds
Published online in Wiley InterScience (www.interscience.wiley.com). DOI:10.1002/aoc.860

Crystallographic report

Di(t-butyl)tin(IV) ester of pyruvic acid isonicotinyl hydrazone

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Received 10 September 2004; Revised 27 September 2004; Accepted 28 September 2004

The tin atom is in a distorted trigonal bipyramidal geometry with the t-butyl groups in equatorial positions within a C_2NO_2 donor set. Copyright © 2005 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; tin; pyruvic acid isonicotinyl hydrazone; carboxylate

COMMENT

Recently, organotin(IV) compounds with Schiff bases have attracted considerable attention owing to their biological activity and diverse structure.[1,2] Two essentially identical independent molecules comprise the asymmetric unit in t-Bu_2Sn[4-$NC_5H_4CONN{=}C(CH_3)COO$]; one molecule is shown in Fig. 1. The tin atom is in a distorted trigonal bipyramidal geometry with the oxygen atoms of the tridentate ligand in axial positions.

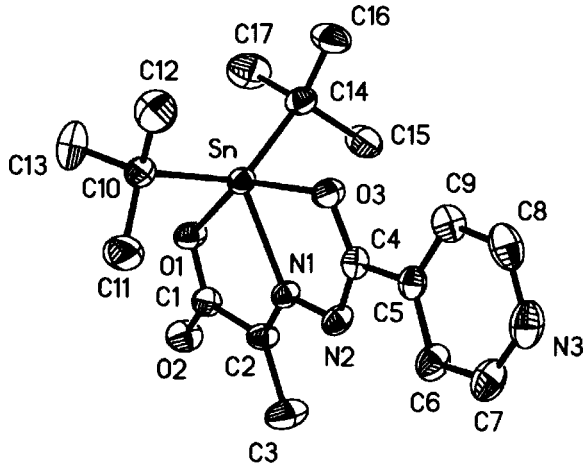

Figure 1. The molecular structure of t-Bu_2Sn[4-$NC_5H_4CONN{=}C(CH_3)COO$]; only one molecule of the asymmetric unit is shown and hydrogen atoms have been omitted for clarity. Key geometric parameters: Sn–O1 2.201(3), Sn–O3 2.246(3), Sn–N1 2.212(4), Sn–C10 2.195(5), Sn–C14 2.184(5) Å; O1–Sn–O3 144.30(12), C10–Sn–C14 132.67(18)°.

EXPERIMENTAL

t-Bu_2Sn[4-$NC_5H_4CONN{=}C(CH_3)COO$] was obtained from the 1 : 1 reaction between t-Bu_2SnCl_2 and the sodium salt of the ligand as per the literature method.[3] Crystals were isolated from the slow evaporation of a C_6H_{14}/CH_2Cl_2 (1 : 4) solution of the compound; m.p. 192 °C. Data were collected at 298(2) K on a Bruker Smart 1000 CCD for a block 0.10 × 0.21 × 0.29 mm^3. $C_{17}H_{25}N_3O_3Sn$, $M = 438.09$, monoclinic, $P2_1/n$, $a = 12.715(3)$, $b = 14.421(3)$, $c = 23.619(5)$ Å, $\beta = 101.301(3)°$, $V = 4247.0(15)$ $Å^3$, $Z = 8$. $R = 0.037$ (4826 data with $I > 2\sigma(I)$; θ_{max} 25.0°), $wR = 0.108$ (all 7422 data). Programs used: SHELXL and ORTEP. CCDC deposition number: 249470.

Acknowledgements

The National Natural Foundation People's Republic of China (20271025) and the National Natural Foundation of Shandong Province are thanked for support.

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Contract/grant sponsor: National Natural Foundation People's Republic of China; Contract/grant number: 20271025.
Contract/grant sponsor: National Foundation of Shandong Province; Contract/grant number: L2003B01.

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