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Crystallographic report

Dicyclopentyltin(IV) bis(2-quinaldinate) methanol solvate

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The tin atom in the title compound is in a skew-trapezoidal bipyramidal geometry defined by two sets of nitrogen and oxygen donors derived from the carboxylate ligands and two carbon atoms from the tin-bound cyclopentyl substituents; C–Sn–C 153.38(16)°. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: tin; quinaldate; carboxylate; crystal structure

COMMENT

A skew-trapezoidal bipyramidal geometry about the tin atom was found in the title structure that was investigated during the study of the structural diversity in these and analogous diorganotin picolinates.[1,2] The geometry reported here (Fig.1) resembles closely those found for other diorganotin quinaldates[1,2] and $^{t}Bu_2Sn$(2-picolinate)$_2$.[3]

EXPERIMENTAL

The title compound was prepared as described in the literature[1,2] and recrystallized by the slow evaporation of methanol solution of the compound, m.p. >260 °C. Intensity data were collected at 173 K on a Rigaku AFC7R diffractometer for a colourless block $0.08 \times 0.10 \times 0.33$ mm^3. $C_{31}H_{31}N_2O_5Sn$, $M = 630.27$, monoclinic, $P2_1/c$, $a = 9.651(2)$, $b = 16.608(5)$, $c = 17.800(3)$ Å, $\beta = 99.45(2)°$, $V = 2814(1)$ Å^3, $Z = 4$, 6459 unique data (θ_{max}27.5°), 3746 data with $I \geq 2\sigma(I)$, $R = 0.034$, (obs. data) $wR = 0.094$ (all data). The methanol molecule of solvation was found to be disordered over two positions; from refinement, these had 50% occupancy each. The molecules were refined isotropically and hydrogen atoms were not included. Programs used: teXsan, DIFABS, DIRDIF, SHELXL-97, and ORTEP. CCDC deposition number: 217674.

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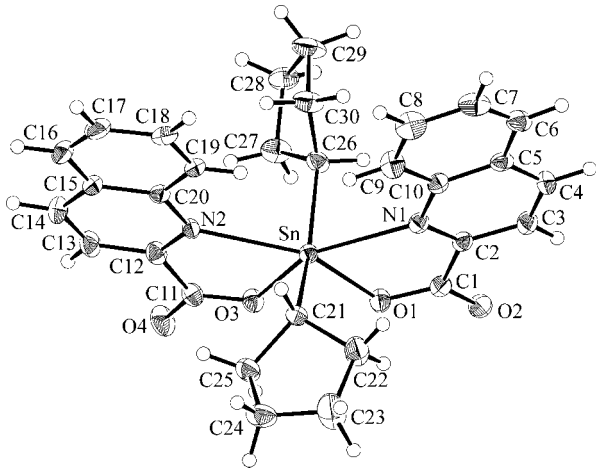

Figure 1. Molecular structure with the methanol molecule of solvation omitted. Key geometric parameters: Sn–O1 2.098(3), Sn–O3 2.104(3), Sn–N1 2.550(3), Sn–N2 2.529(3), Sn–C21 2.140(4), Sn–C26 2.138(4) Å; O1–Sn–O3 79.02(11), N1–Sn–N2 140.64(10), C21–Sn–C26 153.38(16)°.

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