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Crystallographic report

Aquadicylcohexyltin(IV) bis(2-picolinate) ethanol solvate

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The tin atom in the title compound is in a distorted pentagonal bipyramidal geometry defined by two sets of nitrogen and oxygen donors derived from the carboxylate ligands, two carbon atoms from the cyclohexyl substituents and an oxygen atom from the coordinated water molecule; C–Sn–C 170.85(15)°. Extensive hydrogen bonding occurs in the lattice. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: tin; picolinate; carboxylate; crystal structure

COMMENT

The structural diversity in the organotin carboxylates is well documented.[1,2] Amongst these, the structures that show some of the most interesting variations are those containing the 2-picolinate anion.[3–7] In the monomeric title structure (Fig. 1), both 2-picolinate ligands chelate the tin atom via nitrogen and oxygen donors with these plus the tin atom effectively co-planar. A water molecule is also coordinated in this plane, and above and below this are two cyclohexyl groups, so that the overall coordination geometry is based on a pentagonal bipyramid. The water and ethanol molecules interact with the organotin entity through hydrogen bonds. The extensive hydrogen bonding interactions give rise to a chain structure, as found for the analogous methanol solvate.[6,7]

EXPERIMENTAL

The title compound was prepared as described in the literature[6,7] and recrystallized by the slow evaporation of an ethanol/benzene (5:1) solution of the compound, m.p. 226–228 °C. Intensity data were collected at 173 K on a Rigaku AFC7R diffractometer for a tan block 0.13 × 0.16 × 0.40 mm^3. $C_{26}H_{38}N_2O_6Sn$, $M = 593.27$,

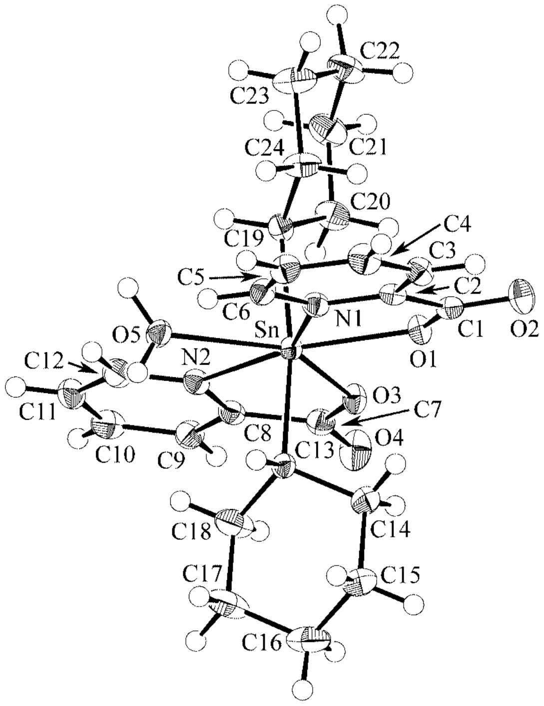

Figure 1. Molecular structure with the ethanol molecule of solvation omitted. Key geometric parameters: Sn–O1 2.232(2), Sn–O3 2.241(3), Sn–O5 2.442(3), Sn–N1 2.540(3), Sn–N2 2.508(3), Sn–C13 2.162(3), Sn–C19 2.158(4) Å; C13–Sn–C19 170.85(15)°.

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monoclinic, *Cc*, $a = 15.871(4)$, $b = 19.92(1)$, $c = 9.835(4)$ Å, $\beta = 123.14(2)°$, $V = 2604(2)$ Å^3, $Z = 4$, 3103 unique data (θ_{max}27.5°), 2781 data with $I \geq 2\sigma(I)$, $R = 0.020$ (obs. data), $wR = 0.048$ (all data); Flack parameter: 0.01(2). Programs used: teXsan, DIFABS, DIRDIF, SHELXL-97, and ORTEP. CCDC deposition number: 217 673.

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REFERENCES

1. Tiekink ERT. *Appl. Organometal. Chem.* 1991; **5**: 1.
2. Tiekink ERT. *Trends Organometal. Chem.* 1994; **1**: 71.
3. Lockhart TP, Davidson F. *Organometallics* 1987; **6**: 2471.
4. Jurkschat K, Tiekink ERT. *Main Group Met. Chem.* 1994; **17**: 659.
5. Gielen M, Bouâlam M, Tiekink ERT. *Main Group Met. Chem.* 1993; **16**: 251.
6. Stapleton CPD. BSc (Hons) thesis, The University of Adelaide, 2000.
7. Dakternieks D, Duthie A, Smyth DR, Stapleton CPD, Tiekink ERT. *Organometallics* 2003; submitted for publication.