APPLIED ORGANOMETALLIC CHEMISTRY, VOL. 8, 37–42 (1994)

Crystal Structure and Fungitoxicity of Aquatributyltin *N*-Phthaloylglycinate

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The [nBu$_3$Sn(*N*-phthaloylglycinate)(OH$_2$)] compound has been prepared and characterized. The crystal structure reveals the tin atom, in each of the two molecules comprising the asymmetric unit, to exist in a distorted trigonal bipyramidal geometry in which the trigonal plane is defined by the three organic substituents and the axial sites are occupied by an oxygen atom derived from a monodentate carboxylate ligand and a coordinated water molecule. The [nBu$_3$Sn(*N*-phthaloylglycinate)(OH$_2$)] compound and three other triorganotin derivatives of *N*-phthaloyl-protected amino acids display marked toxicity against several economically important plant pathogenic fungi.

Keywords: Triorganotin, carboxylate, crystal structure, fungitoxicity

INTRODUCTION

N-Phthaloylglycine condenses readily with a triorganotin hydroxide or hemioxide to form the triorganotin *N*-phthaloylglycinate either as an anhydrous compound or as a hydrate, depending on the nature of the tin-bound organic groups and the reaction medium employed. In boiling ethanol, the *N*-phthaloyl-protected amino acid reacts with triphenyltin hydroxide to give triphenyltin *N*-phthaloylglycinate,[1] but with *p*-chlorophenyldiphenyltin hydroxide it forms the hydrated triorganotin carboxylate (K. M. Low, S. W. Ng and V. G. Kumar Das, unpublished results). The acid affords the anhydrous organotin ester when treated with bis(tributyltin) oxide in boiling toluene[2,3] but the hydrated product resulted when the reagents were melted together. The structure of this hydrate is discussed in this contribution, which also reports some preliminary results on the fungitoxicity of the aquatributyltin *N*-phthaloylglycinate, of the *N*-phthaloylalaninate homologue and of related derivatives.

EXPERIMENTAL

Bis(tributyltin) oxide was melted with *N*-phthaloylglycine (1/2, molar ratio) and the resulting solid was recrystallized from hexane to give aquatributyltin *N*-phthaloylglycinate, m.p. 88–91 °C.

Analysis: Found: C, 51.76; H, 6.94; N, 2.65. Calcd for $C_{22}H_{35}NO_5Sn$: C, 51.59; H, 6.89; N, 2.74%.

Tin-119*m* Mössbauer (80 K): isomer shift (IS) = 1.43, quadrupole splitting (QS) = 3.92, $\Gamma_1 = 1.03$, $\Gamma_2 = 1.01$ mm s^{-1}. Variable-temperature ($80\ \mathrm{K} \leq T \leq 130\ \mathrm{K}$) Mössbauer: $-\mathrm{d}[\ln f(T)]/\mathrm{d}T = 0.0235\ \mathrm{K}^{-1}$ (6 points, $r = -0.996$).

^{1}H NMR data (CDCl$_3$): δ 1.24–1.61 (complex pattern, 18H, —CH$_2$CH$_2$CH$_2$—), 0.87 (triplet, 9H, —CH$_3$), 1.63 (singlet, 2H, OH$_2$), 4.38 (singlet, 2H, —CH$_2$—), 7.71 ppm (quartet, 2H, ═CH), 7.86 (quartet, 2H, ═CH).

^{13}C NMR (CDCl$_3$): δ ($|nJ^{119}\mathrm{Sn}-^{13}\mathrm{C}|$, Hz): C_α 16.6 (350.9), C_β 27.6 (19.7), C_γ 26.9 (62.3), C_δ 13.5 (≤8), $C_{\mathrm{methylene}}$ 39.5, C_{aromatic} 123.3, 132.3, 133.9, C_{carbonyl} 167.7, C_{imido} 171.6 ppm.

For purposes of comparison, bis(tributyltin) oxide was similarly reacted with *N*-phthaloylalanine to afford aquatributyltin *N*-phthaloylalaninate, m.p. 61–65 °C.

Atomic coordinates for this structure have been deposited with the Cambridge Crystallographic Data Centre. The coordinates can be obtained from the Cambridge Crystallographic Data Centre, University Chemical Laboratory, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, UK.

CCC 0268-2605/94/010037-06

Received 22 July 1993
Accepted in revised form 28 October 1993

Analysis: Found: C, 52.65; H, 7.15; N, 2.56. Calcd for $C_{23}H_{37}NO_5Sn$: C, 52.50; H, 7.09; N, 2.66%.

Tin-119*m* Mössbauer (80 K): IS = 1.43, QS = 3.81, $\Gamma_1 = 1.00$, $\Gamma_2 = 1.01$ mm s^{-1}. Variable-temperature ($80\ \mathrm{K} \leq T \leq 130\ \mathrm{K}$) Mössbauer: $-\mathrm{d}[\mathrm{In}\ f(T)]/\mathrm{d}T = 0.0181^{-1}$ K (6 points, $r = -0.996$).

Intensity data for a colourless crystal (0.20 mm × 0.27 mm × 0.43 mm) were measured at −100 ± 1 °C on a Rigaku AFC5R four-circle diffractometer fitted with graphite monochromatized MoKα radiation, $\lambda = 0.71073$ Å. The intensities of three representative reflections which were measured after every 150 reflections decreased by *ca* 7% during the course of the data collection and hence a linear correction factor was applied to the intensity data. A total of 12 127 data were measured (ω: 2θ scan technique and $\theta_{\max}$ was 27.5°), of which 10 126 were unique ($R_{\mathrm{int}} = 0.027$) and 7884 satisfied the $I \geq 3.0\sigma(I)$ criterion of observability and were used in the subsequent analysis. The data were corrected for Lorentz and polarization effects[4] and for absorption employing the DIFABS program[5] which resulted in a range of transmission coefficients of 0.907–1.000.

Crystal data for $C_{22}H_{35}NO_5Sn$: $M = 512.2$, monoclinic, space group $P2_1/n$, $a = 15.022(5)$, $b = 20.201)(5)$, $c = 17.045(6)$ Å, $\beta = 106.75(3)°$, $V = 4953(3)$ Å^3, $Z = 8$, $D_{\mathrm{calcd}} = 1.374$ g cm^{-3}, $F(000) = 2112$, $\mu = 10.61$ cm^{-1}.

The structure was solved by Patterson methods[6] and refined by a full-matrix least-squares procedure based on F.[4] There are two molecules in the crystallographic asymmetric unit and evidence of disorder associated with the butyl groups was found in each of these. The disorder is, in general, not particularly severe, but its presence is reflected in the elongated thermal ellipsoids for some of the atoms in these groups. For one butyl group of each molecule a second position for the β carbon atom was clearly visible in a difference electron density map. The two disordered positions for these atoms were included in the refinement with site occupation factors of 0.75 and 0.25. In order to maintain reasonable bonding geometry within the butyl groups, it was necessary to apply bond length restraints of 1.52 Å to some of the C–C bonds. Non-hydrogen atoms were refined with anisotropic thermal parameters, and hydrogen atoms were included in the model at their calculated positions (C–H, 0.95 Å). At convergence, $R = 0.044$ and $R_w = 0.050$ (sigma weights[4]). The analysis of variance showed no special features and the maximum residual in the final difference map was 0.70 e Å^{-3}. The final fractional atomic coordinates are listed in Table 1 and the crystallographic numbering scheme used is shown in Fig. 1, which was drawn with ORTEP[7] at 50% probability ellipsoids. Data manipulation was performed with the TEXSAN–TEXRAY package[4] installed on a VAX 6320 computer. Other crystallographic details, comprising thermal parameters, hydrogen atom parameters, all bond distances and angles, and tables of observed and calculated structure factors, are available on request from ERTT.

Triphenyltin *N*-phthaloylglycinate, triphenyltin *N*-pthaloylleucinate[1] and the two tributyltin compounds were evaluated *in vitro* for their antifungal activity by the use of the radial growth method.[8] The organotin test solutions were freshly prepared in acetone or 95% ethanol and aseptically added to malt agar extract to give a final concentration of 1–100 µg cm^{-3}. The mixtures were placed in Petri dishes, inoculated with fungal cultures growing on malt agar extract or corn meal agar and then incubated for six days. Colony diameters were taken as the mean of two perpendicular diameters. A probit-log concentration analysis[9] was performed to calculate the effective doses for 50% inhibition of fungal growth (ED_{50}).

DISCUSSION

Bis(tributyltin) oxide condenses with *N*-phthaloylglycine and with *N*-phthaloylalanine in the absence of solvents to yield the monohydrated carboxylates, [nBu$_3$Sn(*N*-phthaloylglycinate)(OH$_2$)] and [nBu$_3$Sn(*N*-phthaloylalaninate)(OH$_2$)], respectively:

$$(Bu_3Sn)_2O + 2HO_2CCH_2\overline{NC(O)C_6H_4C}(O) + H_2O \rightarrow$$

$$2Bu_3SnO_2CCH_2\overline{NC(O)C_6H_4C}(O) \cdot H_2O$$

$$(Bu_3Sn)_2O + 2HO_2CCHMe\overline{NC(O)C_6H_4C}(O) + H_2O \rightarrow$$

$$2Bu_3SnO_2CCHMe\overline{NC(O)C_6H_4C}(O) \cdot H_2O$$

Table 1 Fractional atomic coordinates for [$n\mathrm{Bu_3Sn}$(*N*-phthaloylglycinate)($\mathrm{OH_2}$)]

Molecule **a**				Molecule **b**			
Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
Sn(1)	0.24730(2)	0.23651(1)	0.18055(2)	Sn(2)	0.26649(2)	0.24635(1)	0.70690(2)
O(1)	0.3629(2)	0.1717(1)	0.2430(2)	O(6)	0.3836(2)	0.1848(2)	0.7741(2)
O(2)	0.4787(2)	0.2076(2)	0.1973(2)	O(7)	0.4783(2)	0.2016(2)	0.6973(2)
O(3)	0.5302(2)	0.1656(1)	0.4592(2)	O(8)	0.5408(2)	0.1643(2)	0.9754(2)
O(4)	0.3932(2)	0.0053(2)	0.2760(2)	O(9)	0.4047(2)	0.0127(2)	0.7799(2)
O(5)	0.1167(2)	0.3091(2)	0.1262(2)	O(10)	0.1276(2)	0.3105(2)	0.6452(3)
N(1)	0.4725(2)	0.0917(2)	0.3547(2)	N(2)	0.4866(2)	0.0934(2)	0.8662(2)
C(1)	0.4466(3)	0.1721(2)	0.2410(2)	C(31)	0.4572(3)	0.1753(2)	0.7544(3)
C(2)	0.5108(3)	0.1222(2)	0.2953(3)	C(32)	0.5252(3)	0.1258(2)	0.8086(3)
C(3)	0.4835(3)	0.1177(2)	0.4323(2)	C(33)	0.4918(3)	0.1185(2)	0.9440(3)
C(4)	0.4289(3)	0.0742(2)	0.4714(2)	C(34)	0.4297(3)	0.0758(2)	0.9760(3)
C(5)	0.4174(3)	0.0757(2)	0.5487(3)	C(35)	0.4118(4)	0.0778(2)	1.0510(3)
C(6)	0.3645(3)	0.0257(2)	0.5689(3)	C(36)	0.3511(4)	0.0297(3)	1.0648(3)
C(7)	0.3235(3)	−0.0233(2)	0.5132(3)	C(37)	0.3121(4)	−0.0176(3)	1.0056(4)
C(8)	0.3351(3)	−0.0245(2)	0.4357(3)	C(38)	0.3303(3)	−0.0190(3)	0.9311(3)
C(9)	0.3872(3)	0.0253(2)	0.4159(2)	C(39)	0.3907(3)	0.0291(2)	0.9172(3)
C(10)	0.4140(3)	0.0362(2)	0.3394(2)	C(40)	0.4241(3)	0.0414(2)	0.8457(3)
C(11)	0.2672(4)	0.3010(3)	0.2820(3)	C(41)	0.3404(3)	0.3373(2)	0.7121(3)
C(12)	0.3377(4)	0.2836(3)	0.3620(3)	C(42)	0.3182(3)	0.3876(2)	0.7691(3)
C(13)	0.3428(4)	0.3334(3)	0.4293(3)	C(43)	0.3700(4)	0.4539(3)	0.7727(4)
C(14)	0.4156(5)	0.3161(5)	0.5086(4)	C(44)	0.3392(4)	0.5051(3)	0.8244(4)
C(15)	0.2906(3)	0.2658(2)	0.0768(3)	C(45)	0.2101(4)	0.2318(3)	0.8073(4)
C(16)	0.3509(3)	0.3279(2)	0.0921(3)	C(46)	0.1693(5)	0.1655(3)	0.8152(4)
C(17)	0.3849(4)	0.3461(3)	0.0195(4)	C(47)	0.1418(5)	0.1568(3)	0.8940(4)
C(18)	0.4432(5)	0.4093(3)	0.0344(5)	C(48)	0.0876(7)	0.0943(4)	0.8902(6)
C(19)	0.1505(4)	0.1571(3)	0.1658(5)	C(49)	0.2385(4)	0.1809(3)	0.6070(3)
C(20)[a]	0.1771(4)	0.0946(3)	0.2128(4)	C(50)[a]	0.1685(5)	0.1991(4)	0.5282(3)
C(20A)[b]	0.147(2)	0.0862(4)	0.136(1)	C(50A)[b]	0.228(1)	0.1993(7)	0.5184(4)
C(21)	0.1002(5)	0.0429(3)	0.1858(6)	C(51)	0.1650(5)	0.1506(3)	0.4593(3)
C(22)	0.1283(7)	−0.0109(4)	0.2502(6)	C(52)	0.0865(5)	0.1721(4)	0.3876(4)

[a] Disordered atom with site occupation factor of 0.75. [b] Disordered atom with site occupation factor of 0.25.

The Mössbauer QS values determine a *trans*-trigonal bipyramidal configuration for the five-coordinate tin centres in the compounds. The large slopes of the variable-temperature plots suggest the presence of a weakly associated lattice, with the water molecule being coordinated to the tin atom, rather than a rigid carboxylate-bridged structure with the water molecule in outer-sphere coordination. The slopes are similar to that reported for [$\mathrm{Ph_3Sn}$(8-quinolyl-oxyacetate)($\mathrm{OH_2}$)], which has a helical chain structure in which the monomeric units are held together by hydrogen bonds.[10] The detailed structure of the tributyltin compounds has been afforded by a single-crystal structure analysis of [$n\mathrm{Bu_3Sn}$(*N*-phthaloylglycinate)($\mathrm{OH_2}$)].

The molecular structure of [$n\mathrm{Bu_3Sn}$(*N*-phthaloylglycinate)($\mathrm{OH_2}$)] is shown in Fig. 1 and selected interatomic parameters are listed in Table 2. There are two molecules in the crystallographic asymmetric unit, labelled **a** and **b**, which are distinguished from each other in relatively minor, but experimentally significant, differences in derived interatomic parameters and considerable differences in the relative dispositions of the ligands. The tin atom in each molecule exists in a distorted trigonal bipyramidal geometry with the three organic substituents defining the trigonal plane and the axial positions being occupied by a oxygen atom of a monodentate carboxylate ligand and a water molecule; O(1)–Sn(1)–O(5) and O(6)–Sn(2)–O(10) are 173.7(1) and 172.9(1)°, respectively. The SnO(carboxylate) bond distances are significantly shorter, and experimentally equivalent, at 2.190(3) and 2.189(4) Å for molecules **a** and **b**, respectively, compared with the SnO(water) distances of 2.410(4) and 2.423(4) Å, respectively. The Sn(1) and Sn(2) atoms lie 0.0670(3) and 0.1933(3) Å out of the respective trigonal planes, i.e. in the direction of the O(1) and O(6) atoms; the sum of the C–Sn–C angles is 357.6(7)° for the Sn(1) atom and 359.7(7)° for the Sn(2) centre. The second oxygen atom of each of the carboxylate residues does not make a significant bonding interaction to the tin atom with the Sn(1)···O(2) separation being 3.454(4) Å and Sn(2)···O(7) being 3.356(4) Å. Other differences between the two molecules comprising the asymmetric unit relate to the different orientations of the ligands (see later).

The difference in the secondary Sn–O(carboxylate) interactions probably reflects the different orientations of the carboxylate ligands with respect to the rest of the molecule. An examination of Fig. 1 reveals that there is a twist about the primary Sn–O(carboxylate) vector such that the C(1)–O(1)–Sn(1)–C(15) torsion angle is 26.3(4)° compared with the corresponding angle of −58.3(4)° for C(31)–O(6)–Sn(2)–C(41) (molecule **b**). The relatively close approach and disposition of the O(7) atom relative to the Sn(2) centre open the C(41)–Sn(2)–C(49) angle to 123.7(2)°, which may be contrasted with the regular trigonal angles for molecule **a** (Table 2), drawing the Sn(2) atom above the trigonal plane, i.e. in a direction away from the coordinated water molecule, and consequently it may be concluded that there is greater distortion in the coordination geometry about the Sn(2) atom. The other major difference between the structures is found in the disposition of the n-butyl groups relative to the phthaloyl groups. Using the C(15)–C(18) and C(41)–C(44) n-butyl groups as a reference, in molecule **a** two n-butyl groups are orientated towards the phthaloyl

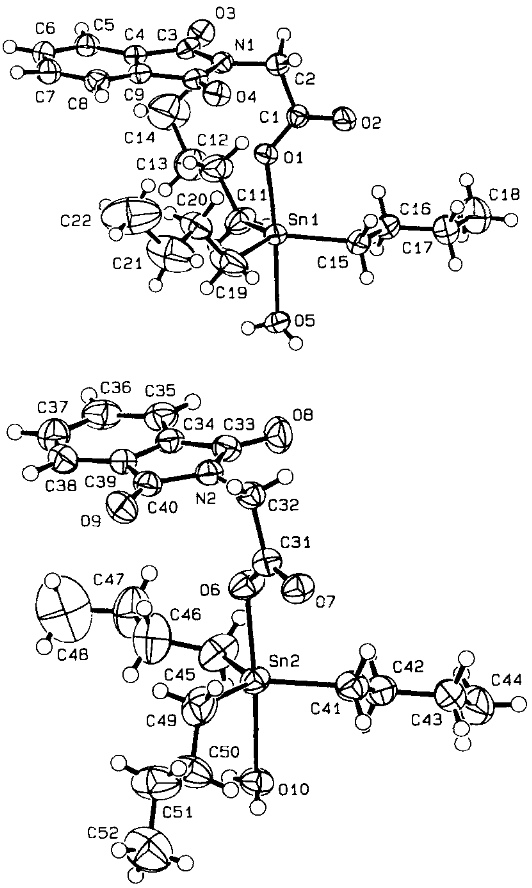

Figure 1 Molecular structure and crystallographic numbering scheme for the two molecules comprising the asymmetric unit in [nBu_3Sn(*N*-phthaloylglycinate)(OH_2)].

Table 2 Selected bond distances (Å) and angles (deg) for [nBu_3Sn(*N*-phthaloylglycinate)(OH_2)]

Atoms	Distance	Atoms	Distance
Sn–O(1)	2.190(3)	Sn(2)–O(6)	2.189(4)
Sn(1)–O(5)	2.410(4)	Sn(2)–O(10)	2.423(4)
Sn(1)–C(11)	2.116(5)	Sn(2)–C(41)	2.135(6)
Sn(1)–C(15)	2.137(5)	Sn(2)–C(45)	2.137(7)
Sn(1)–C(19)	2.131(6)	Sn(2)–C(49)	2.101(6)
O(1)–C(1)	1.267(5)	O(6)–C(31)	1.260(6)
O(2)–C(1)	1.228(6)	O(7)–C(31)	1.227(6)
N(1)–C(2)	1.440(6)	N(2)–C(32)	1.433(7)
C(1)–C(2)	1.513(6)	C(31)–C(32)	1.533(6)

Atoms	Angle	Atoms	Angle
O(1)–Sn(1)–O(5)	173.7(1)	O(6)–Sn(2)–O(10)	172.9(1)
O(1)–Sn(1)–C(11)	93.7(2)	O(6)–Sn(2)–C(41)	97.9(2)
O(1)–Sn(1)–C(15)	100.3(2)	O(6)–Sn(2)–C(45)	87.0(2)
O(1)–Sn(1)–C(19)	91.5(2)	O(6)–Sn(2)–C(49)	90.6(2)
O(5)–Sn(1)–C(11)	81.2(2)	O(10)–Sn(2)–C(41)	86.0(2)
O(5)–Sn(1)–C(15)	85.5(2)	O(10)–Sn(2)–C(45)	86.0(2)
O(5)–Sn(1)–C(19)	87.7(2)	O(10)–Sn(2)–C(49)	92.2(2)
C(11)–Sn(1)–C(15)	120.1(2)	C(41)–Sn(2)–C(45)	114.0(2)
C(11)–Sn(1)–C(19)	119.4(3)	C(41)–Sn(2)–C(49)	123.7(2)
C(15)–Sn(1)–C(19)	118.1(2)	C(45)–Sn(2)–C(49)	122.0(2)
Sn(1)–O(1)–C(1)	129.6(3)	Sn(2)–O(6)–C(31)	125.6(3)
C(2)–N(1)–C(3)	123.2(3)	C(32)–N(2)–C(33)	124.0(4)
C(2)–N(1)–C(10)	124.6(3)	C(32)–N(2)–C(40)	123.5(4)
C(3)–N(1)–C(10)	112.0(4)	C(33)–N(2)–C(40)	111.2(4)
O(1)–C(1)–O(2)	125.8(3)	O(6)–C(31)–O(7)	126.3(4)
O(1)–C(1)–C(2)	116.3(4)	O(6)–C(31)–C(32)	114.9(4)
O(2)–C(1)–C(2)	117.8(4)	O(7)–C(31)–C(32)	118.8(4)
N(1)–C(2)–C(1)	113.7(4)	N(2)–C(32)–C(31)	112.4(4)

group, whereas in molecule **b** one is directed away (see Fig. 1). The reason for this disparity between the structures may be found in the nature of the intermolecular contacts in the lattice.

Hydrogen bonding interactions are known to play a significant role in determining the crystal structures of hydrated organotin compounds, the compounds adopting conformations so that the water molecules form as many hydrogen bonds as possible.[11] Although relatively few aquatriorganotin carboxylates have been structurally characterized,[12] the available data for these compounds show that the coordinated water molecule interacts with the carbonyl oxygen atom and any other basic sites that may be present in the molecule. For example, the water molecule in [Ph$_3$Sn(8-quinolyloxyacetate)(OH$_2$)] is four-coordinate owing to hydrogen-bonding interactions with the carbonyl oxygen, ether oxygen and quinolinyl nitrogen atoms.[10] In the lattice of {nBu$_3$Sn(*N*-phthaloylglycinate)(OH$_2$)], the water molecule of molecule **a** forms hydrogen-bonding contacts with a carbonyl oxygen atom of a symmetry-related molecule **b** [i.e. H(52)· · ·O(7′), 1.97(8), O(5)· · ·O(7′) 2.700(5) Å, O(5)–H(52)· · ·O(7′) 160(8)°; symmetry operation $-0.5+x$, $0.5-y$, $-0.5+z$] and an imido oxygen atom of a neighbouring molecule **a** [i.e. H(51)· · ·O(3′) 2.03(6), O(5)· · ·O(3′) 2.815(5) Å, O(5)–H(51)· · ·O(3′) 170(6)°]. In molecule **b** the water molecule also makes two contacts, again one to a carbonyl oxygen atom [H(101)· · ·O(2″) 1.82(5), O(10)· · ·O(2″) 2.660(5) Å, O(10)–H(101)· · ·O(2″) 152(5)°; symmetry operation: $-0.5+x$, $0.5-y$, $0.5+z$] and the other to an imido oxygen atom [H(102)· · ·O(8″) 2.09(7), O(10)· · ·O(8′) 2.857(5) Å, O(10)–H(102)· · ·O(8′) 158(7)°]. The combination of the two types of hydrogen bonds links the molecules into infinite planes which lie parallel to the crystallographic *ac*-plane; a view of the unit cell contents is shown in Fig. 2.

There are several crystal structures known for compounds of the general formula [R$_3$Sn(O$_2$CR′)L] in which the tin atom exists in a distorted trigonal bipyramidal geometry with the organic substituents defining the trigonal plane and the axial positions are occupied by a monodentate carboxylate ligand and a neutral ligand. Two of the structures, i.e. [Ph$_3$Sn(8-quinolyloxyacetate)(OH$_2$)][10] and [(*p*-ClC$_6$H$_4$)Ph$_2$Sn(*N*-phthaloylglycinate)(OH$_2$)] (K. M. Lo, S. W. Ng and V. G. Kumar Das, unpublished results), feature L = H$_2$O and the other structurally characterized example, i.e. [Ph$_3$Sn(O$_2$CCl$_3$)(CH$_3$OH)], has L = CH$_3$OH.[13]

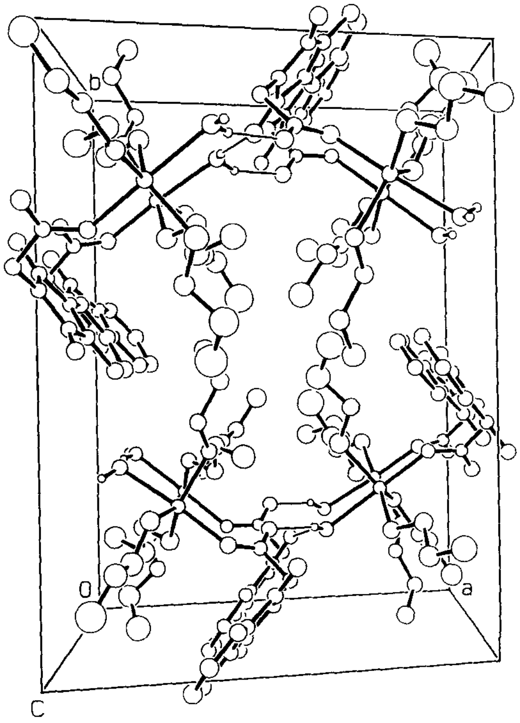

Figure 2 Unit cell contents for [nBu$_3$Sn(*N*-phthaloylglycinate)(OH$_2$)].

In chloroform solution [nBu$_3$Sn(*N*-phthaloylglycinate)(OH$_2$)] dissociates into water and tetrahedral [nBu$_3$Sn(*N*-phthaloylglycinate)], as suggested by the $^1J(^{119}Sn^{13}C)$ value of 350.9 Hz in the ^{13}C NMR spectrum. This value exceeds marginally that (344.4 Hz) measured for [nBu$_3$Sn(2,2-dichloropropionate)], which has a tetrahedral structure in solution.[14]

The antifungal spectra of [nBu$_3$Sn(*N*-phthaloylglycinate)(OH$_2$)], [nBu$_3$Sn(*N*-phthaloylalaninate)(OH$_2$)] and two [Ph$_3$Sn(*N*-phthaloylaminoacetate)] compounds are presented in Table 3; the ED$_{50}$ values have been calculated based on the colony-growth (radial extension) measurements of the test fungus over a six-day period. The ED$_{50}$ values for the tributyltin derivatives generally fall below the 1 ppm range; the ED$_{50}$ values for the triphenyltin derivatives range from 0.22 to 10.00 ppm, which demonstrates that these compounds possess a higher degree of selectivity in their fungitoxic action.

Table 3 ED_{50} values for triorganotin *N*-phthaloylaminoacetates against selected plant-pathogenic fungi[a]

Fungus	**I**	**II**	**III**	**IV**
Alternaria padwickii[b]	0.69	1.21	0.89	9.00
Botryodiplodia theobromae 122[c]	0.42	0.67	2.18	2.06
Colletotrichum musae[d]	0.49	0.68	0.84	1.03
Colletotrichum musae 246[d]	0.81	1.00	1.26	1.71
Colletotrichum musae 273[d]	0.50	0.95	0.84	0.93
Colletotrichum gloeosporiodes 282[c]	1.20	1.58	2.17	2.76
Pestalotiopsis guepini[f]	0.55	0.72	0.22	10.00
Phytophthora palmivora 56[g]	0.70	0.83	1.71	3.07
Phytophthora palmivora 139[g]	0.98	0.95	2.95	5.60
Pyricularia oryzae[h]	0.74	0.94	0.94	0.94

[a] **I**, [nBu_3Sn(*N*-phthaloylglycinate)(OH_2)]; **II**, [nBu_3Sn(*N*-phthaloylalaninate)(OH_2)]; **III**, [Ph_3Sn(*N*-phthaloylglycinate)(OH_2)]; **IV**, [Ph_3Sn(*N*-phthaloylleucinate)(OH_2)]. [b] Causes spoilage of rice in field and on storage. [c] Causes lesions on tropical fruit and vegetables. [f] Causes spoilage of cereal crops and lesions on tropical fruit. [g] Causes foot-rot in petter, black-pod, patch canker and seedling dieback in cocoa. [h] Causes rice blast disease.

The fungitoxicities of the two aqua tributyltin compounds compare well with that of the xanthyl-substituted carboxylate, tributyltin isopropoxyxanthylacetate, which gave an ED_{50} value of 0.69 ppm when screened against *Phytophthora palmivora* 56.[15]

Acknowledgements The Malaysian National Science Council for R&D (2-07-04-06), the University of Malaya (PJP 152/91) and the Australian Research Council are thanked for support.

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