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## Key indicators

Single-crystal X-ray study

T = 298 K

Mean  $\sigma(\text{C}-\text{C}) = 0.012 \text{ \AA}$ 

R factor = 0.037

wR factor = 0.078

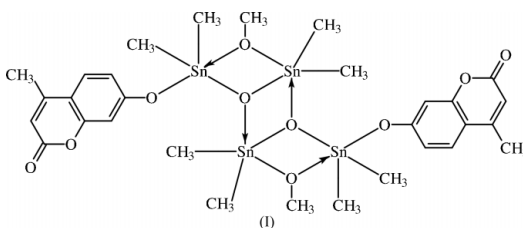
Data-to-parameter ratio = 16.0

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Bis[3-(4-methylcoumarinyl-7-oxy)- $\mu$ -methoxy-1,1,3,3-tetramethyl-distannoxane]

Centrosymmetric bis[3-(4-methylcoumarinyl-7-oxy)- $\mu$ -methoxy-1,1,3,3-tetramethyl-distannoxane],  $[\mu\text{-OCH}_3\text{-(CH}_3)_2\text{(C}_{10}\text{H}_7\text{O}_3\text{)Sn-O-Sn(CH}_3)_2\text{]}_2$ , possesses a central rhombic  $\text{Sn}'_2\text{O}'_2$  core, which is flanked on opposite sides by the  $\text{Sn}'\text{O}'\text{Sn}''\text{O}''$  unit (where  $\text{O}'$  is the distannoxanyl O atom and  $\text{O}''$  is the methoxyl O atom). The two Sn atoms are both five-coordinate, in a *cis*- $\text{C}_2\text{SnO}_3$  trigonal bipyramidal geometry [ $\text{C}-\text{Sn}-\text{C}$  130.6 (4) and 133.3 (4)°].

## Comment

Since the photophysical properties of fluorophores that are complexed with metals are distinctly different from those of the fluorophores themselves (Löhr & Vögtle, 1985; Thanabal & Krishnan, 1982; Tundo & Fendler, 1980; Ghosh *et al.*, 1988), such complexes are of potential application as laser dyes, frequency converters and ion-recognition agents (Bourson & Valeur, 1989; Bourson *et al.*, 1982, 1983; Ernsting *et al.*, 1988). Among the fluoroionophores, the most studied are coumarin derivatives (Bourson & Valeur, 1989); in their complexes, the light-emitting ability is expected to depend on the metal atom itself. Among organotin compounds, derivatives in which the Sn atom is linked, albeit indirectly, to a coumarin entity (Ng, 1999; Ng & Kumar Das, 1997) have also been reported. The present centrosymmetric bis[3-(4-methylcoumarinyl-7-oxy)- $\mu$ -methoxy-1,1,3,3-tetramethyl-distannoxane],  $[\mu\text{-OCH}_3\text{-(CH}_3)_2\text{(C}_{10}\text{H}_7\text{O}_3\text{)Sn-O-Sn(CH}_3)_2\text{]}_2$ , (I) (Fig. 1), is formally a distannoxane; distannoxanes are the hydrolysis products of diorganotin derivatives such as chlorides and carboxylates (Ng *et al.*, 1991).

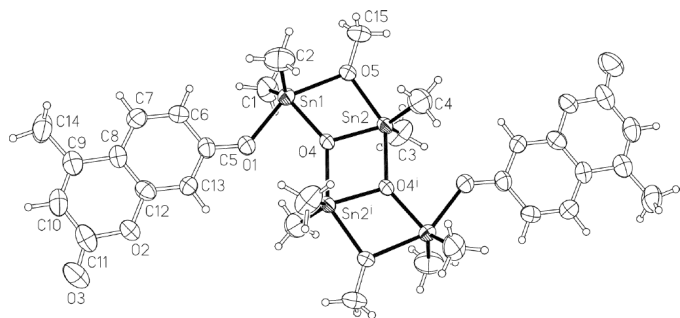


Unlike the dimeric, tetranuclear distannoxanes that are formulated as  $[(R_2\text{Sn}X)_2\text{O}]_2$ , the four  $X$  entities in the present compound are not identical; two are aryloxy and two are methoxy units. Such a 'mixed' distannoxane is unprecedented in organotin chemistry (Haiduc & Edelmann, 1999). The compound features a central rhombic  $\text{Sn}_2\text{O}_4$  core, flanked on opposite sides by the  $\text{Sn}1-\text{O}4-\text{Sn}2-\text{O}5$  unit (where  $\text{O}5$  is the distannoxanyl O atom and  $\text{O}4$  is the methoxyl O atom). The aryloxy group is covalently linked to atom Sn1, which is five-coordinate in a *cis*- $\text{C}_2\text{SnO}_3$  trigonal bipyramidal geometry

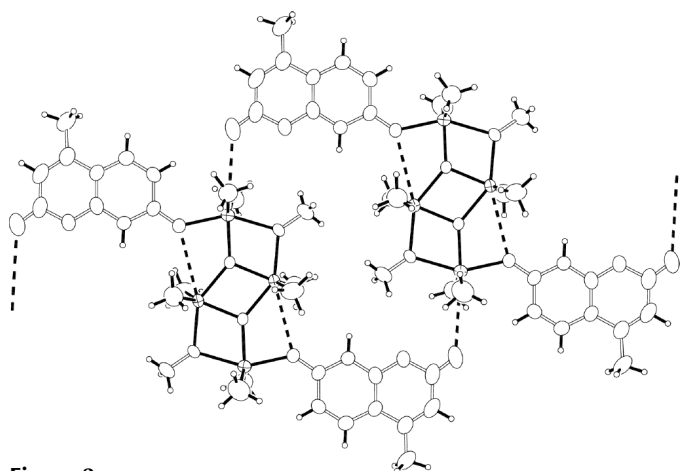
Received 5 September 2003

Accepted 8 September 2003

Online 18 September 2003



**Figure 1**  
ORTEP plot of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii. [Symmetry code (i)  $1 - x, 1 - y, 1 - z$ .]



**Figure 2**  
ORTEP plot of the layer structure. Weak Sn...O interactions are shown as dashed lines.

[C1—Sn1—C2 133.3 (4)°]. Its O atom interacts weakly with atom Sn2, at a distance of approximately 3.3 Å, but the interaction does not widen the C—Sn—C angle [C3—Sn2—C4 130.6 (4)°], so that the geometry of this atom is also a *cis*-C<sub>2</sub>SnO<sub>3</sub> trigonal bipyramid. The entire molecule is nearly flat; adjacent molecules are linked by much weaker Sn...O (> 3.5 Å) interactions, giving rise to a layer structure (Fig. 2).

In methanol solution, the compound shows a UV absorption maximum at 324 nm (molar extinction coefficient 29,000 M<sup>-1</sup> cm<sup>-1</sup>); the free organic reagent also absorbs at this wavelength (Abdel-Mottaleb *et al.*, 1989). The fluorescence quantum yield is significantly higher (0.83 compared with 0.42 for the coumarin). Although the maximum absorption band is sufficiently near the peak lasing wavelength of a nitrogen laser that can be used as the pump source, the compound is not sufficiently soluble for its lasing action to be ascertained. For commercially available laser dyes, this concentration is typically 10<sup>-4</sup> to 10<sup>-3</sup> M.

## Experimental

Dimethyltin oxide (0.83 g, 5 mmol) and 7-hydroxy-4-methylcoumarin (1.74 g, 10 mmol) were heated in methanol (10 ml) for several hours until most of the oxide had dissolved. The solvent was removed and

the compound recrystallized from a 1/1 CH<sub>2</sub>Cl<sub>2</sub>/CH<sub>3</sub>OH mixture to furnish crystals that melt at temperatures higher than 573 K.

## Crystal data

[Sn<sub>2</sub>(C<sub>10</sub>H<sub>7</sub>O<sub>3</sub>)<sub>2</sub>(CH<sub>3</sub>O)<sub>2</sub>(CH<sub>3</sub>)<sub>8</sub>O<sub>2</sub>]  
*M<sub>r</sub>* = 1039.41  
 Triclinic, *P* $\bar{1}$   
*a* = 8.811 (3) Å  
*b* = 9.717 (3) Å  
*c* = 12.724 (4) Å  
 $\alpha$  = 104.87 (4)°  
 $\beta$  = 93.42 (4)°  
 $\gamma$  = 115.266 (7)°  
*V* = 934.2 (5) Å<sup>3</sup>

*Z* = 1  
*D<sub>x</sub>* = 1.848 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 22 reflections  
 $\theta$  = 3.0–9.9°  
 $\mu$  = 2.69 mm<sup>-1</sup>  
*T* = 298 (2) K  
 Plate, colorless  
 0.20 × 0.20 × 0.04 mm

## Data collection

Siemens *P4* four-circle diffractometer  
 $\omega$ -2 $\theta$  scans  
 Absorption correction:  $\psi$  scan (North *et al.*, 1968)  
*T<sub>min</sub>* = 0.642, *T<sub>max</sub>* = 0.898  
 3983 measured reflections  
 3287 independent reflections  
 2285 reflections with *I* > 2σ(*I*)

*R<sub>int</sub>* = 0.032  
 $\theta_{\max}$  = 25.0°  
*h* = -1 → 10  
*k* = -11 → 10  
*l* = -15 → 15  
 3 standard reflections every 97 reflections  
 intensity decay: 8.7%

## Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.037  
*wR*(*F*<sup>2</sup>) = 0.078  
*S* = 0.99  
 3287 reflections  
 205 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0271P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.54 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.54 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

Sn1—C1	2.087 (8)	Sn2—C3	2.108 (8)
Sn1—C2	2.11 (1)	Sn2—C4	2.077 (9)
Sn1—O1	2.101 (5)	Sn2—O4	2.024 (5)
Sn1—O4	1.998 (5)	Sn2—O4 <sup>i</sup>	2.088 (4)
Sn1—O5	2.223 (5)	Sn2—O5	2.157 (5)
C1—Sn1—C2	133.3 (4)	C3—Sn2—O4 <sup>i</sup>	97.4 (3)
C1—Sn1—O1	97.5 (3)	C3—Sn2—O5	97.1 (3)
C1—Sn1—O4	113.1 (3)	C4—Sn2—O4	116.1 (4)
C1—Sn1—O5	92.8 (3)	C4—Sn2—O4 <sup>i</sup>	98.4 (3)
C2—Sn1—O1	98.8 (4)	C4—Sn2—O5	95.7 (3)
C2—Sn1—O4	112.7 (4)	O4—Sn2—O4 <sup>i</sup>	73.0 (2)
C2—Sn1—O5	93.4 (4)	O4—Sn2—O5	72.3 (2)
O1—Sn1—O4	79.9 (2)	O4 <sup>i</sup> —Sn2—O5	145.3 (2)
O4—Sn1—O5	71.4 (2)	Sn1—O4—Sn2	114.9 (2)
O1—Sn1—O5	151.3 (2)	Sn1—O4—Sn2 <sup>i</sup>	138.0 (2)
C3—Sn2—C4	130.6 (4)	Sn2—O4—Sn2 <sup>i</sup>	107.0 (2)
C3—Sn2—O4	113.3 (4)		

Symmetry codes: (i)  $1 - x, 1 - y, 1 - z$ .

The carbon-bound H atoms were positioned geometrically and treated as riding on the parent C atoms (C—H 0.93 Å and *U*<sub>iso</sub> = 1.2*U*<sub>eq</sub>C for the aromatic H atoms; C—H 0.96 Å and *U*<sub>iso</sub> = 1.5*U*<sub>eq</sub>(C) for the methyl H atoms). The torsion angles of the methyl groups were refined.

Data collection: *XSCANS* (Bruker, 1997); cell refinement: *LEAST SQUARES* in *XSCANS*; data reduction: *REDUCE* in *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

The authors thank the Ministry of Science, Technology and the Environment, Malaysia (IRPA 09-02-03-0662), Nanyang Technological University and the University of Malaya for supporting this work.

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