

Jens Beckmann,\*‡ Dainis Dakternieks, Andrew Duthie and Cassandra Mitchell

Centre for Chiral and Molecular Technologies,  
Deakin University, Geelong 3217, Victoria,  
Australia

‡ Present address: Institut für Chemie, Freie  
Universität Berlin, Fabeckstrasse 34–36, 14195  
Berlin, Germany.

Correspondence e-mail:  
beckmann@chemie.fu-berlin.de

Key indicators

Single-crystal X-ray study  
T = 293 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.008 \text{ \AA}$   
R factor = 0.054  
wR factor = 0.111  
Data-to-parameter ratio = 22.4

For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

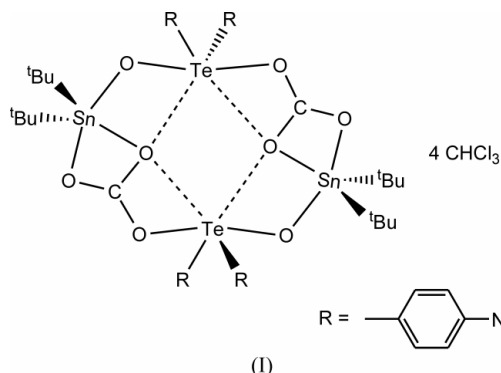
A dimeric tellurastannoxane carbonate cluster,  
tetra-tert-butyl-di- $\mu_3$ -carbonato-tetrakis-  
[4-(N,N-dimethylamino)phenyl]di- $\mu$ -oxo-  
ditelluriumditin chloroform tetrasolvate

The title compound,  $[\text{Sn}_2\text{Te}_2(\text{C}_4\text{H}_9)_4(\text{CO}_3)_2\text{O}_2(\text{C}_8\text{H}_{10}\text{N})_4] \cdot 4\text{CHCl}_3$  or  $[(p\text{-Me}_2\text{NC}_6\text{H}_4)_2\text{TeOSn}^t\text{Bu}_2\text{CO}_3]_2 \cdot 4\text{CHCl}_3$ , contains an almost planar centrosymmetric inorganic  $\text{Sn}_2\text{Te}_2\text{O}_8\text{C}_2$  core and hypercoordinated Sn and Te atoms. The structure features four secondary intramolecular  $\text{Te} \cdots \text{O}$  contacts.

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Comment

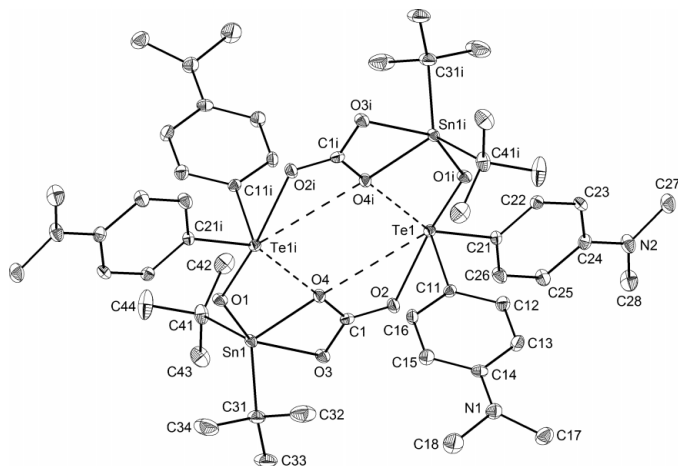
The title compound,  $[(p\text{-Me}_2\text{NC}_6\text{H}_4)_2\text{TeOSn}^t\text{Bu}_2\text{CO}_3]_2 \cdot 4\text{CHCl}_3$ , (I), is a close analogue of the recently published compound  $[(p\text{-MeOC}_6\text{H}_4)_2\text{TeOSn}^t\text{Bu}_2\text{CO}_3]_2$ , (II), and was formed when a solution of  $(^t\text{Bu}_2\text{SnO})_3$  and  $(p\text{-Me}_2\text{N}-\text{C}_6\text{H}_4)_2\text{TeO}$  (Sn:Te ratio = 1:1) was purged with an excess of carbon dioxide (Beckmann *et al.*, 2004).



The centrosymmetric structure of (I) (Fig. 1 and Table 1) features an almost planar  $\text{Sn}_2\text{Te}_2\text{C}_2\text{O}_8$  core, the largest deviation from the mean plane being  $0.461(15) \text{ \AA}$  for atom Te1. The geometry of the Sn atom is distorted trigonal bipyramidal and is defined by a  $\text{C}_2\text{O}_3$  donor set. The distortion appears to originate from the chelating coordination mode of the carbonate moiety. When considering the primary and secondary coordination spheres, but not the stereochemically active lone pair, the geometry of the Te atom is strongly distorted octahedral, defined by a  $\text{C}_2\text{O}_2 + \text{O}_2$  donor set.

The most striking feature of the structure of (I) is the network of four (two independent) secondary  $\text{Te} \cdots \text{O}$  interactions [ $3.159(3)$  and  $3.255(3) \text{ \AA}$ ], which seem to contribute to the configurational stability of the cluster. The three C—O bond lengths of the carbonate group are rather different [ $1.252(6)$ ,  $1.282(6)$  and  $1.326(6) \text{ \AA}$ ], which presumably stems from the varying donation of electron density of the O atoms to the Sn and Te atoms, respectively.

The absorption of gaseous carbon dioxide by the two organometallic oxides ('fixation') and the discrepancy of the



**Figure 1**

A view of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. Chloroform molecules and all H atoms have been omitted for clarity. [Symmetry code as in Table 1].

C—O bond lengths ('bond activation') suggest applications of (I) as a recyclable C1 feedstock for commodity chemicals, such as urea and dimethyl carbonate (DMC).

## Experimental

Compound (I) was prepared in a manner analogous to that used for [(*p*-MeOC<sub>6</sub>H<sub>4</sub>)<sub>2</sub>TeOSn<sup>i</sup>Bu<sub>2</sub>CO<sub>3</sub>]<sub>2</sub>, (II) (Beckmann *et al.*, 2004), and obtained in yield of 95%. Crystals (m.p. 501–503 K) were grown from a solution in chloroform (100 mg ml<sup>-1</sup>) at room temperature. Analysis calculated for C<sub>50</sub>H<sub>76</sub>N<sub>4</sub>O<sub>8</sub>Sn<sub>2</sub>Te<sub>2</sub> (*M<sub>r</sub>*, 1353.78): C 44.36, H 5.66%; found: C 44.44, H 5.67%. Spectroscopic analysis: <sup>1</sup>H NMR (299.98 MHz, CDCl<sub>3</sub>, δ, p.p.m.): 1.17 [*s*, <sup>2</sup>*J*(<sup>1</sup>H–<sup>117/119</sup>Sn)] 105, 36H, 'Bu', 2.96 (*d*, 24H, NMe<sub>2</sub>), 6.68 (*d*, 8H, C<sub>6</sub>H<sub>4</sub>), 7.94 (*s*, 8H, C<sub>6</sub>H<sub>4</sub>); <sup>13</sup>C{<sup>1</sup>H} NMR (75.44 MHz, CDCl<sub>3</sub>, δ, p.p.m.): 29.36 ('Bu), 38.95 ('Bu), 40.16 (NMe<sub>2</sub>), 112.40 (C<sub>6</sub>H<sub>4</sub>), 124.34 (C<sub>6</sub>H<sub>4</sub>), 133.27 (C<sub>6</sub>H<sub>4</sub>), 151.74 (C<sub>6</sub>H<sub>4</sub>), 165.36 (CO<sub>3</sub>); <sup>119</sup>Sn{<sup>1</sup>H} NMR (100.73 MHz, CDCl<sub>3</sub>, δ, p.p.m.): –257.9; <sup>119</sup>Sn MAS NMR (149.10 MHz, δ<sub>iso</sub>, p.p.m.): –267.5; <sup>125</sup>Te{<sup>1</sup>H} NMR (85.34 MHz, CDCl<sub>3</sub>, δ, p.p.m.): 1213.2; <sup>125</sup>Te MAS NMR (126.27 MHz, δ<sub>iso</sub>, p.p.m.): 1195.4.

### Crystal data

[Sn<sub>2</sub>Te<sub>2</sub>(C<sub>4</sub>H<sub>9</sub>)<sub>4</sub>(CO<sub>3</sub>)<sub>2</sub>O<sub>2</sub>–  
(C<sub>8</sub>H<sub>10</sub>N)<sub>4</sub>·4CHCl<sub>3</sub>]  
*M<sub>r</sub>* = 1831.20  
Monoclinic, *P*2<sub>1</sub>/*c*  
*a* = 11.0573 (8) Å  
*b* = 14.4144 (10) Å  
*c* = 23.1203 (17) Å  
β = 96.946 (1)°  
*V* = 3658.0 (5) Å<sup>3</sup>  
*Z* = 2

*D<sub>x</sub>* = 1.663 Mg m<sup>-3</sup>  
Mo *K*α radiation  
Cell parameters from 4050  
reflections  
θ = 2.3–25.9°  
μ = 1.95 mm<sup>-1</sup>  
*T* = 293 (2) K  
Rod, colourless  
0.50 × 0.15 × 0.10 mm

### Data collection

Bruker SMART CCD area-detector  
diffractometer  
φ and ω scans  
Absorption correction: multi-scan  
(*SADABS*; Bruker, 2000)  
*T<sub>min</sub>* = 0.681, *T<sub>max</sub>* = 0.823  
22 007 measured reflections

8301 independent reflections  
6590 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.048  
θ<sub>max</sub> = 27.5°  
*h* = –14 → 13  
*k* = –18 → 18  
*l* = –30 → 15

### Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.055  
*wR* [*F*<sup>2</sup>] = 0.111  
*S* = 1.09  
8301 reflections  
370 parameters  
H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0434P)^2 + 5.0552P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
(Δ/*σ*)<sub>max</sub> < 0.001  
Δρ<sub>max</sub> = 1.25 e Å<sup>-3</sup>  
Δρ<sub>min</sub> = –1.30 e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Sn1—O1	2.040 (3)	Te1—O2	2.501 (4)
Sn1—O3	2.313 (3)	Te1—C11	2.097 (5)
Sn1—O4	2.085 (3)	Te1—C21	2.112 (5)
Sn1—C31	2.157 (6)	C1—O2	1.252 (6)
Sn1—C41	2.157 (5)	C1—O3	1.282 (6)
Te1—O1 <sup>i</sup>	1.918 (3)	C1—O4	1.326 (6)
C1—O2—Te1	116.1 (3)	C31—Sn1—C41	130.7 (2)
C1—O3—Sn1	88.5 (3)	O1 <sup>i</sup> —Te1—O2	174.14 (13)
C1—O4—Sn1	97.7 (3)	O1 <sup>i</sup> —Te1—C11	94.36 (18)
O1—Sn1—O3	147.58 (13)	O1 <sup>i</sup> —Te1—C21	90.64 (17)
O1—Sn1—O4	88.12 (14)	O2—Te1—C11	82.95 (16)
O3—Sn1—O4	59.50 (13)	O2—Te1—C21	84.54 (16)
O1—Sn1—C31	98.05 (18)	C11—Te1—C21	97.10 (19)
O1—Sn1—C41	101.25 (19)	Te1 <sup>i</sup> —O1—Sn1	126.49 (18)
O3—Sn1—C31	93.88 (18)	O2—C1—O3	123.7 (5)
O3—Sn1—C41	93.35 (18)	O2—C1—O4	122.0 (5)
O4—Sn1—C31	113.03 (19)	O3—C1—O4	114.3 (5)
O4—Sn1—C41	112.51 (19)		

Symmetry code: (i) 1 – *x*, 1 – *y*, –*z*.

The H atoms were placed in geometrically calculated positions and refined using a riding model, with primary C—H = 0.96, secondary C—H = 0.97 and tertiary C—H = 0.93 Å, and with *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C) for non-methyl H atoms and 1.5*U*<sub>eq</sub>(C) for methyl groups. The highest peak and deepest hole are 0.92 Å from C11 and 0.94 Å from H34C, respectively.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Bergerhoff *et al.*, 1996); software used to prepare material for publication: *SHELXL97*.

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## References

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