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# Diaquadichlorodiphenyltin(IV) 18-crown-6

**Mostafa M. Amini,[a] Amirreza Azadmeher,[a] Mohammad Yousefi,[b] Shahrbano Foladi[b] and Seik Weng Ng[c]***

[a]Department of Chemistry, Shahid Beheshti University, Tehran, Iran, [b]Department of Chemistry, Science and Research Campus, Islamic Azad University, Tehran, Iran, and [c]Institute of Postgraduate Studies, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail:
h1nswen@umcsd.um.edu.my

**Key indicators**

Single-crystal X-ray study
*T* = 168 K
Mean $\sigma$(C–C) = 0.004 Å
*R* factor = 0.028
*wR* factor = 0.069
Data-to-parameter ratio = 16.7

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

Diaquadichlorodiphenyltin(IV) 18-crown-6, $[SnCl_2(C_6H_5)_2(H_2O)_2]\cdot C_{12}H_{24}O_6$, adopts an all-*trans* octahedral configuration at the Sn atom. The coordinated water molecule forms a pair of hydrogen bonds to the polyether to furnish a linear hydrogen-bonded chain structure. There are two half-molecules of each component in the asymmetric unit, with the Sn atoms and the centres of the crown ethers lying on inversion centres.

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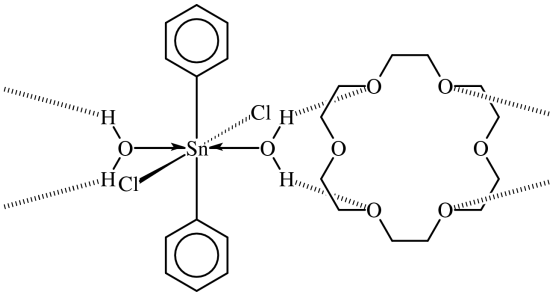
## Comment

Diorganotin dichlorides react with 18-crown-6 to furnish complexes in which the Sn atom interacts indirectly, through a coordinated water molecule, with the crown ether. Dimethyltin dichloride forms a monohydrate having the formulation $(CH_3)_2SnCl_2\cdot H_2O\cdot\frac{1}{2}C_{12}H_{24}O_6$. The adduct features an unusual environment of water: the water molecules are engaged in twin three-centre hydrogen bonds, and the structure represents the first example of such an arrangement (Amini *et al.*, 1984). A later account of the methylphenyltin dichloride analogue described a similar motif (Amini *et al.*, 1994). With diphenyltin dichloride, this crown ether yields a dihydrated 1:1 complex in which the diorganotin skeleton has been assigned a linear configuration on the basis of the $^{119m}$Sn Mössbauer quadrupole splitting (Smith & Patel, 1983). This feature is confirmed in the present crystallographic analysis.



(I)

The asymmetric unit of the title compound, (I), exists as two symmetry-independent halves of $(C_6H_5)_2SnCl_2\cdot 2H_2O\cdot$18-crown-6 moieties (Fig. 1), with the Sn atoms located on a centre of inversion; in each of them, the coordinated water molecule forms a pair of hydrogen bonds to two ether O atoms of the crown ether. The hydrogen-bonding interactions lead to the formation of a linear chain structure (Fig. 2). The parent Lewis acid, diphenyltin dichloride, exists as two independent tetrahedral molecules [Sn—C = 2.105 (5)–2.119 (5) Å; Sn—

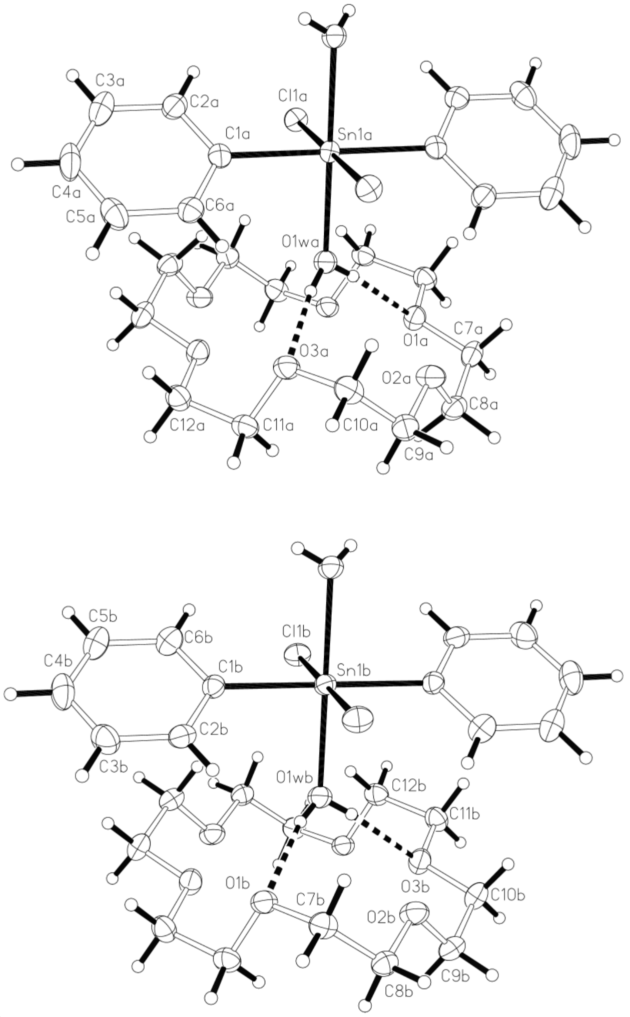


**Figure 1**
*ORTEP* (Johnson, 1976) plots of molecules *a* (top) and *b* (bottom) with displacement ellipsoids shown at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

Cl = 2.336 (2)–2.357 (2) Å; Greene & Bryan, 1971]. Coordination of the water molecules to the Sn atom does not alter the Sn—C distances; however, the Sn—Cl distance is lengthened by about 10% in the title complex.

## Experimental

The title compound was synthesized by the reaction of diphenyltin dichloride and 18-crown-6 in methanol (Smith & Patel, 1983). The reagents, in a 1:1 molar stoichiometry, were heated in the solvent; the product that deposited upon removal of the solvent was recrystallized from acetonitrile.

### *Crystal data*

$[SnCl_2(C_6H_5)_2(H_2O)_2]\cdot C_{12}H_{24}O_6$
$M_r$ = 644.13
Triclinic, $P\overline{1}$
$a$ = 8.0970 (6) Å
$b$ = 12.355 (1) Å
$c$ = 14.701 (1) Å
$\alpha$ = 84.116 (2)°
$\beta$ = 82.041 (3)°
$\gamma$ = 75.302 (3)°
$V$ = 1405.4 (2) Å$^3$
$Z$ = 2
$D_x$ = 1.522 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 4783 reflections
$\theta$ = 1.7–26.4°
$\mu$ = 1.14 mm$^{-1}$
$T$ = 168 (2) K
Plate, colourless
0.49 × 0.25 × 0.04 mm

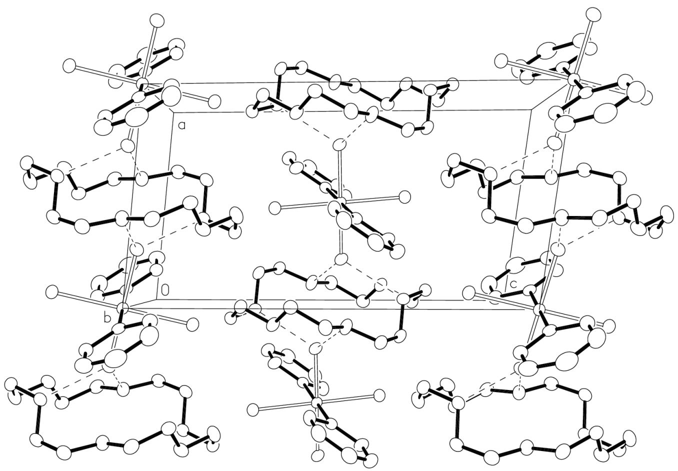


**Figure 2**
*ORTEP*II (Johnson, 1976) plot showing the hydrogen-bonded chain structure. H atoms are not shown.

### *Data collection*

Siemens CCD area-detector diffractometer
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\rm min}$ = 0.605, $T_{\rm max}$ = 0.956
17544 measured reflections
5523 independent reflections
4296 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.030
$\theta_{\rm max}$ = 26.4°
$h = -9 \rightarrow 5$
$k = -15 \rightarrow 15$
$l = -18 \rightarrow 18$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.069
$S$ = 1.04
5523 reflections
331 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0355P)^2 + 0.3568P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max}$ = 0.77 e Å$^{-3}$
$\Delta\rho_{\rm min}$ = −0.62 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Sn1*a*—C1*a* | 2.159 (3) | Sn1*b*—C1*b* | 2.160 (3) |
| Sn1*a*—O1*wa* | 2.253 (2) | Sn1*b*—O1*wb* | 2.262 (2) |
| Sn1*a*—Cl1*a* | 2.5521 (7) | Sn1*b*—Cl1*b* | 2.5627 (7) |
| | | | |
| C1*a*—Sn1*a*—C1*a*$^{\rm i}$ | 180.0 | C1*b*—Sn1*b*—C1*b*$^{\rm ii}$ | 180.0 |
| C1*a*—Sn1*a*—O1*wa* | 90.03 (9) | C1*b*—Sn1*b*—O1*wb* | 89.49 (9) |
| C1*a*—Sn1*a*—O1*wa*$^{\rm i}$ | 89.97 (9) | C1*b*—Sn1*b*—O1*wb*$^{\rm ii}$ | 90.51 (9) |
| C1*a*—Sn1*a*—Cl1*a* | 89.72 (7) | C1*b*—Sn1*b*—Cl1*b* | 90.07 (7) |
| C1*a*—Sn1*a*—Cl1*a*$^{\rm i}$ | 90.28 (7) | C1*b*—Sn1*b*—Cl1*b*$^{\rm ii}$ | 89.93 (7) |
| O1*wa*—Sn1*a*—O1*wa*$^{\rm i}$ | 180.0 | O1*wb*—Sn1*b*—O1*wb*$^{\rm ii}$ | 180.0 |
| O1*wa*—Sn1*a*—Cl1a | 89.87 (5) | O1*wb*—Sn1*b*—Cl1*b* | 90.31 (5) |
| O1*wa*$^{\rm i}$—Sn1*a*—Cl1*a* | 90.13 (5) | O1*wb*—Sn1*b*—Cl1*b*$^{\rm ii}$ | 89.69 (5) |
| Cl1*a*—Sn1*a*—Cl1*a*$^{\rm i}$ | 180.0 | Cl1*b*—Sn1*b*—Cl1*b*$^{\rm ii}$ | 180.0 |

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

**Table 2**
Hydrogen-bonding geometry (Å, °).

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| O1*wa*—H1*a*1$\cdots$O1*a* | 0.84 (1) | 2.00 (1) | 2.823 (3) | 165 (3) |
| O1*wa*—H1*a*2$\cdots$O3*a* | 0.84 (1) | 1.93 (1) | 2.766 (3) | 172 (3) |
| O1*wb*—H1*b*1$\cdots$O1*b* | 0.84 (1) | 2.02 (1) | 2.842 (3) | 165 (3) |
| O1*wb*—H1*b*2$\cdots$O3*b* | 0.84 (1) | 2.11 (2) | 2.891 (3) | 155 (3) |

*Acta Cryst.* (2002). E**58**, m58–m60 Mostafa M. Amini *et al.* • $[SnCl_2(C_6H_5)_2(H_2O)_2]\cdot C_{12}H_{24}O_6$ **m59**

The water H atoms were located and refined, subject to O—H = 0.85±0.01 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(O). Other H atoms were constrained.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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