Table 1. *Fractional atomic coordinates and B_{eq} values* (Å^2)

$B_{eq} = 8\pi^2(U_{11} + U_{22} + U_{33})/3.$

	x	y	z	B_{eq}
Sn	0·27553 (2)	0·10188 (2)	0·19474 (2)	4·07
O(1)	0·3028 (3)	0·2527 (3)	0·0593 (3)	5·01
O(2)	0·2596 (5)	0·4142 (3)	0·1789 (4)	6·26
O(3)	0·2976 (6)	0·5952 (2)	0·0005 (4)	7·29
C(1)	0·2872 (4)	0·3709 (4)	0·0820 (4)	4·36
C(2)	0·3044 (4)	0·4630 (3)	−0·0207 (3)	4·16
C(3)	0·3109 (6)	0·6547 (4)	−0·1094 (5)	6·80
C(4)	0·3233 (6)	0·5682 (4)	−0·1918 (5)	6·01
C(5)	0·3230 (5)	0·4408 (5)	−0·1333 (4)	5·53
C(6)	0·3255 (8)	−0·0448 (5)	0·0736 (6)	7·46
C(7)	0·4400 (5)	0·1666 (6)	0·3517 (5)	6·27
C(8)	0·0639 (5)	0·1432 (6)	0·1725 (6)	6·75

Table 2. *Interatomic distances* (Å) *and bond angles* (°)

Primed atoms are related by $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$.

Sn—O(1)	2·191 (3)	Sn—C(6)	2·138 (5)
Sn—C(7)	2·129 (5)	Sn—C(8)	2·130 (5)
Sn—O(2′)	2·430 (4)	Sn—O(2)	3·175 (4)
Sn—O(3)	3·584 (4)	C(1)—O(1)	1·244 (5)
C(1)—O(2)	1·240 (5)	C(1)—C(2)	1·502 (5)
C(2)—O(3)	1·365 (4)	C(2)—C(5)	1·306 (5)
C(3)—O(3)	1·377 (6)	C(3)—C(4)	1·283 (7)
C(4)—C(5)	1·440 (6)		
O(1)—Sn—C(6)	88·7 (2)	O(1)—Sn—C(7)	96·1 (2)
O(1)—Cn—C(8)	95·5 (2)	O(1)—Sn—O(2′)	172·4 (2)
C(6)—Sn—C(7)	116·2 (3)	C(6)—Sn—C(8)	118·0 (3)
C(6)—Sn—O(2′)	84·2 (2)	C(7)—Sn—C(8)	124·6 (2)
C(7)—Sn—O(2′)	89·7 (2)	C(8)—Sn—O(2′)	85.3 (2)
Sn—O(1)—C(1)	119·6 (2)	Sn—O(2′)—C(1′)	149·9 (3)
O(1)—C(1)—O(2)	125·5 (4)	O(1)—C(1)—C(2)	114·0 (3)
O(2)—C(1)—C(2)	120·6 (4)	C(1)—C(2)—O(3)	117·6 (3)
C(1)—C(2)—C(5)	131·5 (4)	O(3)—C(2)—C(5)	110·8 (4)
C(2)—O(3)—C(3)	105·2 (3)	O(3)—C(3)—C(4)	110·8 (4)
C(3)—C(4)—C(5)	107·1 (4)	C(4)—C(5)—C(2)	106·0 (4)

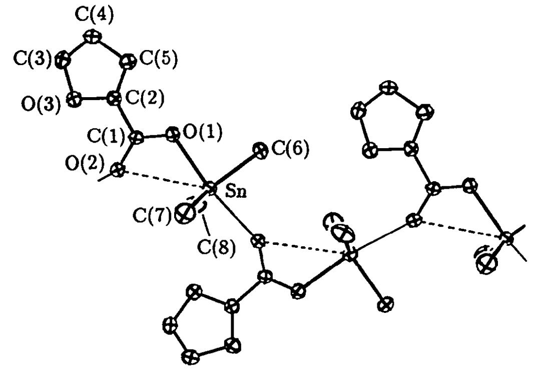

Fig. 1. Molecular structure and numbering scheme for $[Me_3Sn(O_2CC_4H_3O)]_n$ (Johnson, 1971).

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Structure of *trans*-Dichlorotetrakis(diphenylphosphine)ruthenium(II) Chloroform (1/2)

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Abstract. $[RuCl_2(C_{12}H_{11}P)_4].2CHCl_3$, $M_r = 1155·7$, triclinic, $P\bar{1}$, $a = 10·4314\ (11)$, $b = 10·5379\ (28)$, $c = 13·2413\ (8)$ Å, $\alpha = 70·106\ (13)$, $\beta = 73·208\ (7)$, $\gamma = 77·191\ (13)$°, $V = 1298·0$ Å^3, $Z = 1$, $D_x = 1·460$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 0·865$ mm^{-1}, $F(000) = 586$, $T = 298$ K, $R = 0·0311$ for 3154 unique observed reflections. The Ru occupies a crystallographic inversion centre and is octahedrally coordinated by the resulting *trans* arrangement of the ligands.

Experimental. Compound prepared by isomerization of the corresponding *cis* complex in chloroform solution on standing in air, crystals obtained by partial evaporation of this solution. Pale-yellow ingot, 0·6 × 0·4 × 0·3 mm, CAD-4 diffractometer, graphite-monochromated Mo $K\alpha$ radiation, cell parameters by least-squares refinement on diffractometer angles

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Table 1. *Atomic coordinates with e.s.d.'s and isotropic thermal parameters*

$$U_{eq} = \tfrac{1}{3}\textstyle\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}/U_{iso}(Å^2)
Ru	0·0000	0·0000	0·0000	0·02918 (24)
P(1)	−0·13685 (7)	0·20997 (7)	−0·00095 (7)	0·0349 (5)
H(31)	−0·070 (3)	0·314 (3)	−0·062 (3)	0·0800
P(2)	−0·01471 (8)	0·03077 (8)	−0·18207 (6)	0·0357 (5)
H(41)	0·1078 (23)	0·018 (4)	−0·248 (3)	0·0800
Cl(1)	0·18880 (7)	0·12867 (8)	−0·09829 (6)	0·0430 (5)
C(1)	−0·1279 (3)	0·36237 (23)	0·13247 (23)	0·077 (3)
C(2)	−0·1701 (3)	0·40346 (23)	0·22794 (23)	0·110 (5)
C(3)	−0·2756 (3)	0·34772 (23)	0·31299 (23)	0·1223 (5)
C(4)	−0·3391 (3)	0·25088 (23)	0·30257 (23)	0·093 (4)
C(5)	−0·2969 (3)	0·20979 (23)	0·20709 (23)	0·063 (3)
C(6)	−0·1913 (3)	0·26554 (23)	0·12204 (23)	0·0471 (22)
C(7)	−0·33772 (23)	0·39820 (18)	−0·09041 (21)	0·070 (3)
C(8)	−0·45835 (23)	0·43862 (18)	−0·12548 (21)	0·090 (4)
C(9)	−0·53340 (23)	0·34086 (18)	−0·11944 (21)	0·079 (3)
C(10)	−0·48781 (23)	0·20267 (18)	−0·07833 (21)	0·074 (3)
C(11)	−0·36718 (23)	0·16225 (18)	−0·04326 (21)	0·0553 (25)
C(12)	−0·29213 (23)	0·26002 (18)	−0·04930 (21)	0·0412 (21)
C(13)	−0·20119 (22)	−0·14118 (24)	−0·15371 (15)	0·058 (3)
C(14)	−0·26011 (22)	−0·22012 (24)	−0·18903 (15)	0·073 (3)
C(15)	−0·20661 (22)	−0·23769 (24)	−0·29363 (15)	0·082 (4)
C(16)	−0·09418 (22)	−0·17632 (24)	−0·36291 (15)	0·078 (3)
C(17)	−0·03526 (22)	−0·09738 (24)	−0·32759 (15)	0·063 (3)
C(18)	−0·08876 (22)	−0·07981 (24)	−0·22299 (15)	0·0454 (22)
C(19)	−0·18940 (19)	0·22025 (18)	−0·30712 (18)	0·0511 (23)
C(20)	−0·23448 (19)	0·34983 (18)	−0·36995 (18)	0·063 (3)
C(21)	−0·16407 (19)	0·45836 (18)	−0·39304 (18)	0·063 (3)
C(22)	−0·04857 (19)	0·43732 (18)	−0·35329 (18)	0·056 (3)
C(23)	−0·00349 (19)	0·30774 (18)	−0·29047 (18)	0·0455 (22)
C(24)	−0·07391 (19)	0·19920 (18)	−0·26738 (18)	0·0372 (19)
Cl(2)	−0·67819 (12)	0·13620 (13)	−0·45444 (10)	0·0891 (9)
Cl(3)	−0·45929 (12)	0·07484 (13)	−0·34803 (13)	0·1043 (11)
Cl(4)	−0·59500 (14)	0·34822 (12)	−0·40950 (14)	0·1123 (12)
C(25)	−0·6129 (4)	0·1764 (4)	−0·3637 (3)	0·062 (3)

Table 2. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s*

Ru—P(1)	2·3505 (8)	P(1)—C(12)	1·8172 (25)
Ru—P(2)	2·3665 (8)	P(2)—C(18)	1·8217 (24)
Ru—Cl(1)	2·4317 (8)	P(2)—C(24)	1·8331 (23)
P(1)—C(6)	1·812 (3)		

P(1)—Ru—P(2)	90·34 (3)	H(41)—P(2)—C(18)	97·1 (15)
P(1)—Ru—Cl(1)	87·13 (3)	H(41)—P(2)—C(24)	96·2 (15)
P(2)—Ru—Cl(1)	82·00 (3)	C(18)—P(2)—C(24)	101·30 (11)
Ru—P(1)—H(31)	111·8 (14)	P(1)—C(6)—C(1)	120·55 (21)
Ru—P(1)—C(6)	120·73 (10)	P(1)—C(6)—C(5)	119·45 (21)
Ru—P(1)—C(12)	122·76 (8)	P(1)—C(12)—C(7)	119·18 (18)
H(31)—P(1)—C(6)	95·2 (14)	P(1)—C(12)—C(11)	120·80 (18)
H(31)—P(1)—C(12)	101·3 (14)	P(2)—C(18)—C(13)	121·04 (17)
C(6)—P(1)—C(12)	100·18 (12)	P(2)—C(18)—C(17)	118·89 (17)
Ru—P(2)—H(41)	110·8 (15)	P(2)—C(24)—C(19)	120·86 (16)
Ru—P(2)—C(18)	125·27 (8)	P(2)—C(24)—C(23)	119·13 (16)
Ru—P(2)—C(24)	120·29 (8)		

for 25 centred reflections with $28 < 2\theta < 30°$. For data collection, ω–2θ scans with ω-scan width $(0{\cdot}80 + 0{\cdot}35\tan\theta)°$, $2\theta_{max} = 45°$, h $-10\rightarrow11$, k $-10\rightarrow11$, l $0\rightarrow14$, isotropic decay (*ca* 40%) corrected for during processing, no absorption correction, 3386 unique reflections, giving 3154 with $F > 2\sigma(F)$ for structure solution (from a Patterson synthesis followed by iterative cycles of least-squares refinement and difference Fourier synthesis) and refinement [using full-matrix least squares on F (Sheldrick, 1976)]. Anisotropic thermal parameters for all non-H atoms, H atoms in fixed, calculated positions except for those directly bound to P(1) and P(2) where the bonds were constrained to be 1·33 (2) Å. The phenyl rings were refined as planar, idealized hexagons, d(C—C) = 1·395 Å. At final convergence, $R = 0{\cdot}0311$, $wR = 0{\cdot}0448$, $S = 2{\cdot}259$ for 244 parameters, $(\Delta/\sigma)_{max}$ in final cycle 0·021, max. peak and min. trough in final ΔF synthesis 0·31 and $-0{\cdot}39$ e Å^{-3} respectively. The weighting scheme $w^{-1} = \sigma^2(F) + 0{\cdot}000179F^2$ gave satisfactory agreement analyses. Scattering factors were inlaid (Sheldrick, 1976) except for those for Ru (Cromer & Mann, 1968). Atomic coordinates are given in Table 1, while selected bond lengths and angles appear in Table 2.* The atom-numbering scheme for the molecule is shown in Fig. 1, which was generated using *ORTEP* (Mallinson & Muir, 1985). Molecular geometry calculations were performed using *CALC* (Gould & Taylor, 1985).

Related literature. The Ru—P [2·3508 (8), 2·3665 (8) Å] and Ru—Cl [2·4317 (8) Å] distances in the title compound are similar to those found in the corresponding *trans*-$[RuCl_2(Me_2PH)_4]$ (Cotton. Frenz & Hunter, 1976).

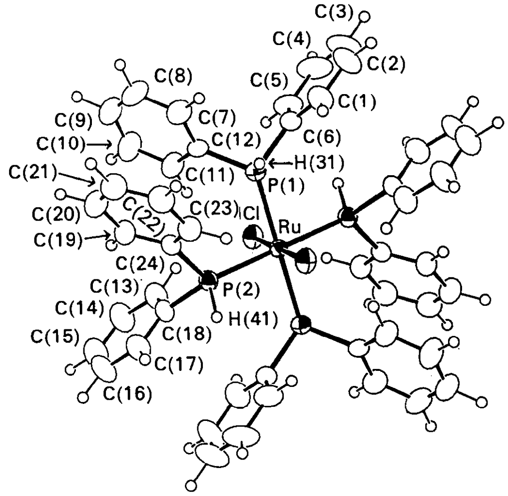

Fig. 1. A general view of the molecule showing atom-numbering scheme: thermal ellipsoids are drawn at the 30% probability level, excepting those of H which have artificial radii of 0·10 Å for clarity. The Ru occupies a crystallographic inversion centre.

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* Lists of structure factors, anisotropic thermal parameters, torsion angles and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51971 (23 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Two Crystal Modifications of Hexamethylcyclotristannatellurane

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Abstract. $[(CH_3)_2SnTe]_3$, $C_6H_{18}Sn_3Te_3$, $M_r = 829{\cdot}1$, Mo $K\alpha$ radiation, $\lambda = 0{\cdot}71069$ Å, $T = 293$ K: (1) monoclinic, $P2_1/c$, $a = 14{\cdot}681$ (2), $b = 10{\cdot}2775$ (8), $c = 13{\cdot}561$ (3) Å, $\beta = 112{\cdot}087$ (12)°, $V = 1896{\cdot}0$ Å^3, $Z = 4$, $D_x = 2{\cdot}905$ Mg m^{-3}, $\mu = 8{\cdot}45$ mm^{-1}, $F(000) = 1439{\cdot}9$, $R = 0{\cdot}034$ for 1968 observed data; (2) tetragonal, $I4_1/a$, $a = 12{\cdot}710$ (3), $c = 22{\cdot}757$ (4) Å, $V = 3676{\cdot}3$ Å^3, $Z = 8$, $D_x = 2{\cdot}996$ Mg m^{-3}, $\mu = 8{\cdot}72$ mm^{-1}, $F(000) = 2879{\cdot}8$, $R = 0{\cdot}024$ for 1507 observed data. In each form the molecule adopts a twist-boat conformation which, in the case of the tetragonal modification, displays crystallographic twofold symmetry.

Experimental. $[(CH_3)_2SnTe]_3$ was obtained in petroleum solution by Soxhlet extraction of the crude reaction product (Blecher & Dräger, 1979; Gay, Jones & Sharma, 1989). Evaporation of the solvent at room temperature yielded a sample consisting mainly of thin yellow-green sheets and a few thicker plates of amber colour. The solid state ^{119}Sn and ^{125}Te NMR spectra (Gay *et al.*, 1989) displayed multiple resonances suggesting that more than one crystalline form was present. A plate selected from this sample for X-ray analysis was found to have crystallized in the space group $P2_1/c$. A different yellow crystal modification was formed exclusively when a saturated petroleum solution of $[(CH_3)_2SnTe]_3$ was cooled to 255 K, as confirmed by its solid state ^{119}Sn and ^{125}Te NMR spectra (Gay *et al.*, 1989). X-ray analysis showed these crystals to be tetragonal, space group $I4_1/a$. Attempts to convert this phase to the monoclinic form by heating were unsuccessful. At 343 K the solid material appeared to fuse to give an apparently polymeric material of negligible solubility in petroleum ether. In either case the crystals became black upon exposure to air for several mintues.

Crystals were mounted on Pyrex filaments with five-minute epoxy resin and were protected from air exposure by a thin coating of resin. Cell-parameter determination (25 reflections $15{\cdot}1 \le \theta \le 19{\cdot}1°$, $P2_1/c$; 24 reflections $20{\cdot}3 \le \theta \le 25{\cdot}7°$, $I4_1/a$) and data acquisition were performed using an Enraf–Nonius CAD-4F diffractometer with Mo $K\alpha$ radiation and a graphite monochromator. The symmetry of the intensity-weighted reciprocal lattices and the systematic absences were determined using the diffractometer. Two standard intensities were measured every hour of acquisition time and showed no systematic variations.

An empirical absorption correction (North, Phillips & Mathews, 1968) was applied to the data in the case of the $I4_1/a$ modification because the irregular shape of the crystal made measurement of crystal faces impracticable. The correction factors applied to the intensities ranged from 1·0 to 0·813. In the $P2_1/c$ case, an analytical absorption correction (de Meulenaer & Tompa, 1965) was made (transmission coefficients ranging from 0·614 to 0·248). Data reduction, including Lorentz and polarization corrections, was performed.

In both cases the coordinates for the Te and Sn atoms were determined by direct methods (Main, Woolfson & Germain, 1971). The C-atom positions were revealed by electron density difference Fourier syntheses. H atoms were fixed at calculated positions with assigned isotropic temperature factors, basing the rotational conformation of each CH_3 group upon the positions of the strongest peaks near the C atoms from a difference Fourier map. The final, full-matrix least-squares refinement, minimizing

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