

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Bis(triphenylphosphanylidene)iminium dichloridotriphenylstannate(IV)

Lucio De Lorentiis, Claudia Graiff* and Giovanni Predieri

Dipartimento di Chimica GIAF, Viale delle Scienze, 17/A, Università di Parma, 43100 Parma, Italy

Correspondence e-mail: claudia.graiff@unipr.it

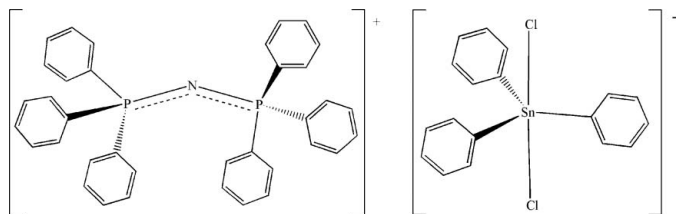
Received 14 July 2011; accepted 30 August 2011

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.025; wR factor = 0.065; data-to-parameter ratio = 26.3.

The structure of the title compound, $[\text{Ph}_3\text{P}=\text{N}=\text{PPh}_3]^+[\text{Ph}_3\text{SnCl}_2]^-$ or $(\text{C}_{36}\text{H}_{30}\text{NP}_2)[\text{Sn}(\text{C}_6\text{H}_5)_3\text{Cl}_2]$, obtained as a by product of the reaction between Ph_3SnCl and $[\text{Ph}_3\text{P}=\text{N}=\text{PPh}_3]^+\cdot\text{HSeO}_3^-$, consists of discrete essentially isolated ions. Both the cation and the anion lie on twofold axes which pass through the central N atom in the cation and through the Sn^{IV} atom in the anion. In the crystal, the ions interact only through a weak interaction between the Cl atom of the anion and an H atom of a phenyl ring of the cation.

Related literature

For general background to selenite compounds, see: Delferro *et al.* (2010, 2011). For related structures, see: Harrison *et al.* (1978); Nayek *et al.* (2010); Ng (1995, 1999). For details of the Cambridge Crystal Structure Database, see: Allen (2002).



Experimental

Crystal data

 $(\text{C}_{36}\text{H}_{30}\text{NP}_2)[\text{Sn}(\text{C}_6\text{H}_5)_3\text{Cl}_2]$ $M_r = 959.44$ Orthorhombic, $Pnn2$ $a = 17.9119$ (6) Å $b = 9.7744$ (3) Å $c = 13.3835$ (4) Å $V = 2343.16$ (13) Å³ $Z = 2$ Mo $K\alpha$ radiation
 $\mu = 0.76$ mm⁻¹ $T = 296$ K
 $0.42 \times 0.22 \times 0.18$ mm

Data collection

Bruker APEXII CCD
diffractometer
Absorption correction: multi-scan
(*SADABS*; Bruker, 2007)
 $T_{\text{min}} = 0.629$, $T_{\text{max}} = 0.746$ 36432 measured reflections
7179 independent reflections
6352 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.025$
 $wR(F^2) = 0.065$
 $S = 1.04$
7179 reflections
273 parameters
1 restraintH-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.20$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.25$ e Å⁻³
Absolute structure: Flack (1983),
3430 Friedel pairs
Flack parameter: -0.022 (13)

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|-------|-------------|-------------|---------------|
| $\text{C9}-\text{H9}\cdots\text{Cl1}^{\dagger}$ | 0.93 | 2.79 | 3.718 (2) | 173 |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Financial support from the PRIN 2008-Molecular Clusters in Nanoscience and the University of Parma, Italy, is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2296).

References

- Allen, F. H. (2002). *Acta Cryst.* **B58**, 380–388.
 Bruker (2007). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Delferro, M., Graiff, C., Elviri, L. & Predieri, G. (2010). *Dalton Trans.* **39**, 4479–4481.
 Delferro, M., Graiff, C., Marchiò, L., Elviri, L., Mazzani, M., Riccò, M. & Predieri, G. (2011). *Eur. J. Inorg. Chem.* doi:10.1002/ejic.201100385.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
 Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
 Harrison, P. G., Molloy, K., Phillips, R. C., Smith, P. J. & Crowe, A. J. (1978). *J. Organomet. Chem.* **160**, 421–434.
 Nayek, H. P., Massa, W. & Dehnen, S. (2010). *Inorg. Chem.* **49**, 144–149.
 Ng, S. W. (1995). *Acta Cryst.* **C51**, 1124–1125.
 Ng, S. W. (1999). *Acta Cryst.* **C55**, IUC9900098.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supporting information

Acta Cryst. (2011). E67, m1356 [https://doi.org/10.1107/S1600536811035422]

Bis(triphenylphosphanylidene)iminium dichloridotriphenylstannate(IV)**Lucio De Lorentiis, Claudia Graiff and Giovanni Predieri****S1. Comment**

The title compound was isolated from a dichloromethane solution as a by product of the reaction between of Ph_3SnCl with $[\text{Ph}_3\text{P}=\text{N}=\text{PPh}_3]^+ \text{HSeO}_3^-$ in dichloromethane solvent. The hydrogen selenite salt, prepared in the framework of our research activity on selenite compounds (Delferro *et al.*, 2010, Delferro *et al.*, 2011), contained a significant amount of $[\text{Ph}_3\text{P}=\text{N}=\text{PPh}_3]^+ \text{Cl}^-$, which is responsible of the formation of the title compound.

The structure of the title compound consists of discrete $[\text{Ph}_3\text{P}=\text{N}=\text{PPh}_3]^+$ and $[\text{Ph}_3\text{SnCl}_2]^-$ ions (Fig. 1). The $[\text{Ph}_3\text{P}=\text{N}=\text{PPh}_3]^+$, (or PPN^+ for simplicity), cation is rather typical, lying on a two fold axis that passes through the central N atom, N1. The P1—N1 bond distance of 1.5763 (9) Å and the P1—N1—P1ⁱ [symmetry code (i) = $-x + 2, -y + 1, z$] bond angle of 141.9 (2)° are in good agreement with the average values of 1.577 (6) Å and 143 (9)° found in 1409 PPN^+ cations reported in the Cambridge Crystal Structure Database (CSD, V5.32, last update May 2011; Allen, 2002), see Fig. 3. In particular, examining the 1409 PPN^+ cations it is evident that less than 40 examples present a linear geometry at the nitrogen atom. On excluding these cases the mean value of the P—N—P bond angle is reduced to 142 (7)°, even more in agreement with the angle in the title compound. The P atom is tetrahedral, with the C—P—C and C—P—N angles averaging 109 (3)°.

The $[\text{Ph}_3\text{SnCl}_2]^-$ anion exhibits trigonal bipyramidal geometry at the tin atom, with the usual equatorial arrangement of organic groups and the chlorine atoms occupying axial positions. The anion is lying on a two-fold axis passing through the tin atom and atom C25 and C28 of one phenyl ring. The C11—Sn1 bond distance is 2.5858 (4) Å and the Cl—Sn—Clⁱⁱ [symmetry code: (ii) = $-x + 2, -y + 2, z$] bond angle is 177.83 (4)°, both in agreement with the values found in four examples (Ng, 1995,1999; Harrison *et al.*, 1978; Nayek *et al.*, 2010) reported in the CSD: The mean values are 2.590 (2) Å and 176.6 (7)°, respectively. The mean planes of the phenyl rings form dihedral angles of 59.70 (2)° and 38.78 (2)° with the SnC_3 mean plane.

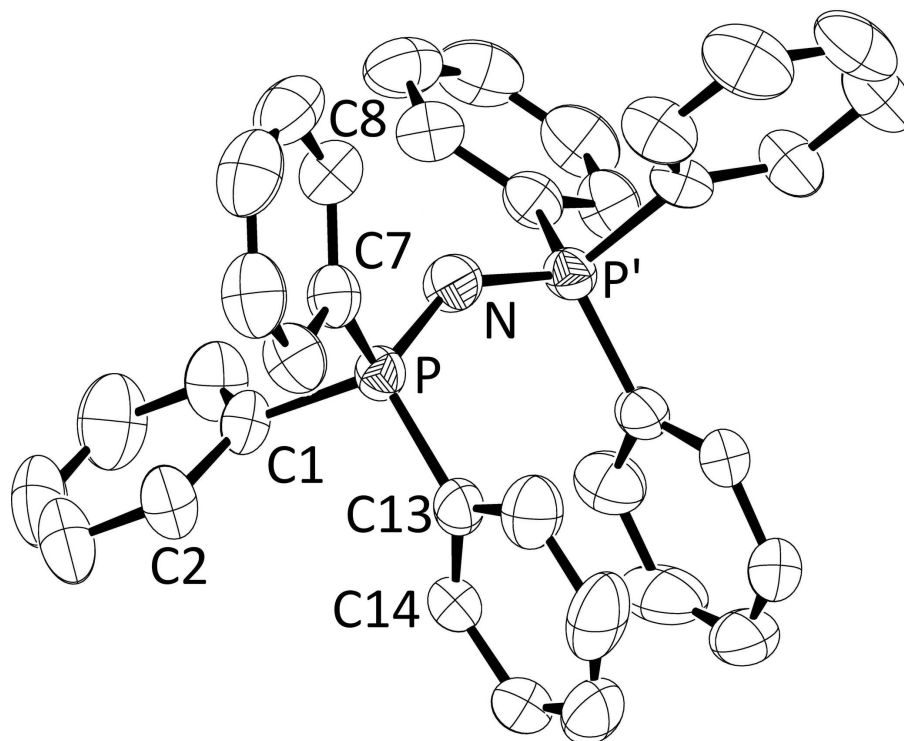
In the crystal there is a weak interaction between the chlorine atom of the dichlorotriphenylstannate anion and a hydrogen atom of a phenyl ring of the bis(triphenylphosphine)iminium cation (Table 1).

S2. Experimental

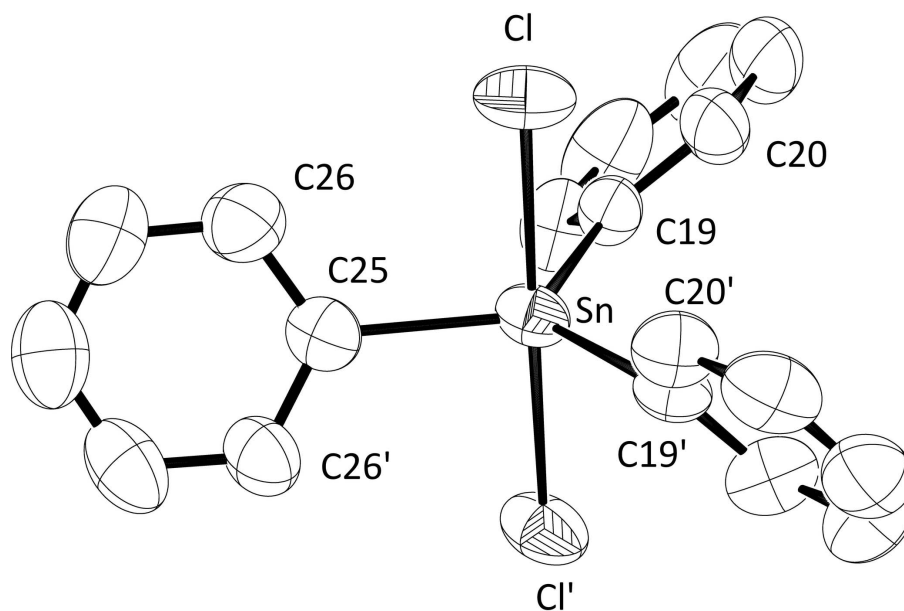
A dichloromethane solution of equimolar amounts of triphenyl-tin chloride and bis(triphenylphosphine)iminium hydrogenselenite was stirred at room temperature for 1 h. The solution was then cooled slowly to 278 K. Crystals suitable for X-ray analysis were obtained from the solution in two days.

S3. Refinement

The C-bound H-atoms were included in calculated positions and treated as riding atoms: C-H = 0.93 Å for CH(aromatic), with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{parent C-atom})$.

**Figure 1**

ORTEP drawing of the $[\text{Ph}_3\text{P}=\text{N}=\text{PPh}_3]^+$ cation, showing the atom labelling and the displacement ellipsoids drawn at the 30% probability level. Hydrogen atoms are omitted for clarity. Symmetry code for generating equivalent atoms: ' = $-x + 2, -y + 1, z$.

**Figure 2**

ORTEP drawing of the $[\text{Ph}_3\text{SnCl}_2]^-$ anion, showing the atom labelling and the displacement ellipsoids drawn at the 30% probability level. Hydrogen atoms are omitted for clarity. Symmetry code for generating equivalent atoms: ' = $-x + 2, -y + 2, z$.

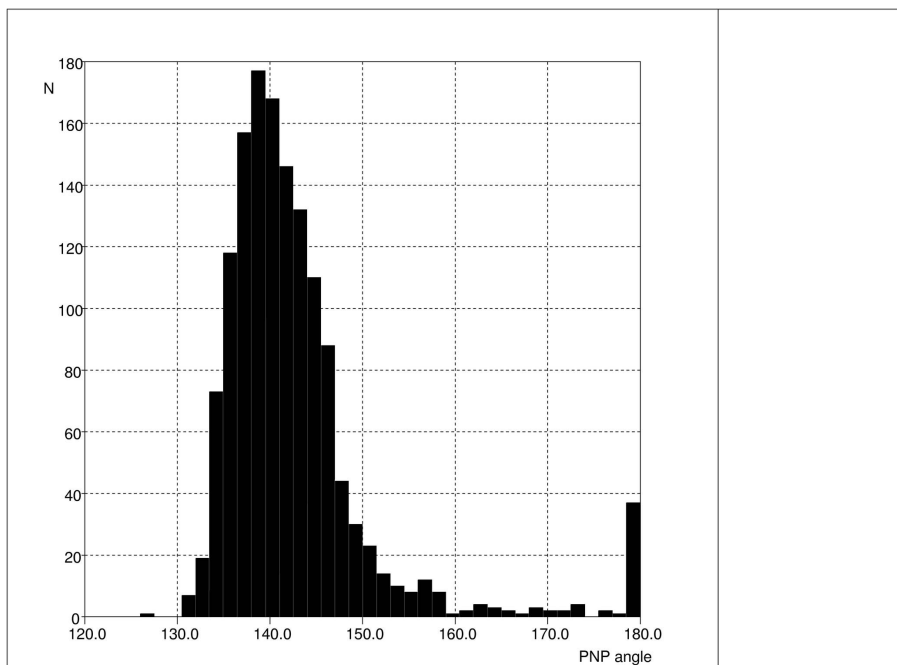


Figure 3

Histogram showing the distribution of the P—N—P bond angle over the 1409 $[\text{Ph}_3\text{P}=\text{N}=\text{PPh}_3]^+$ cations reported in the Cambridge Structural Database (Allen, 2002).

Bis(triphenylphosphanylidene)iminium dichloridotriphenylstannate(IV)

Crystal data

$(\text{C}_{36}\text{H}_{30}\text{NP}_2)[\text{Sn}(\text{C}_6\text{H}_5)_3\text{Cl}_2]$

$M_r = 959.44$

Orthorhombic, $Pnn2$

Hall symbol: $P\ 2\ -2n$

$a = 17.9119\ (6)\ \text{\AA}$

$b = 9.7744\ (3)\ \text{\AA}$

$c = 13.3835\ (4)\ \text{\AA}$

$V = 2343.16\ (13)\ \text{\AA}^3$

$Z = 2$

$F(000) = 980$

$D_x = 1.360\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 999 reflections

$\theta = 3\text{--}27^\circ$

$\mu = 0.76\ \text{mm}^{-1}$

$T = 296\ \text{K}$

Prism, colourless

$0.42 \times 0.22 \times 0.18\ \text{mm}$

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2007)

$T_{\min} = 0.629$, $T_{\max} = 0.746$

36432 measured reflections

7179 independent reflections

6352 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$

$\theta_{\max} = 30.6^\circ$, $\theta_{\min} = 1.9^\circ$

$h = -25 \rightarrow 25$

$k = -13 \rightarrow 13$

$l = -19 \rightarrow 19$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.025$ $wR(F^2) = 0.065$ $S = 1.04$

7179 reflections

273 parameters

1 restraint

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0339P)^2 + 0.062P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 0.20 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.25 \text{ e } \text{\AA}^{-3}$ Absolute structure: Flack (1983), **3430 Friedel
pairs**Absolute structure parameter: -0.022 (13)*Special details*

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|--------------|----------------------------------|
| C1 | 0.88435 (9) | 0.69033 (16) | 0.54090 (12) | 0.0432 (3) |
| C2 | 0.81206 (10) | 0.72511 (17) | 0.51192 (17) | 0.0576 (5) |
| H2 | 0.7811 | 0.6596 | 0.4832 | 0.069* |
| C3 | 0.78656 (12) | 0.8566 (2) | 0.5259 (2) | 0.0726 (6) |
| H3 | 0.7384 | 0.8800 | 0.5065 | 0.087* |
| C4 | 0.83185 (16) | 0.9526 (2) | 0.5683 (2) | 0.0786 (7) |
| H4 | 0.8146 | 1.0416 | 0.5764 | 0.094* |
| C5 | 0.90228 (15) | 0.9193 (2) | 0.5988 (2) | 0.0812 (7) |
| H5 | 0.9323 | 0.9852 | 0.6287 | 0.097* |
| C6 | 0.92925 (11) | 0.7871 (2) | 0.58522 (17) | 0.0611 (5) |
| H6 | 0.9772 | 0.7643 | 0.6059 | 0.073* |
| C7 | 0.85781 (9) | 0.40724 (16) | 0.59273 (12) | 0.0436 (3) |
| C8 | 0.88264 (11) | 0.3604 (2) | 0.68448 (15) | 0.0542 (4) |
| H8 | 0.9306 | 0.3818 | 0.7060 | 0.065* |
| C9 | 0.83627 (14) | 0.2816 (2) | 0.74452 (16) | 0.0677 (5) |
| H9 | 0.8530 | 0.2500 | 0.8061 | 0.081* |
| C10 | 0.76534 (13) | 0.2506 (2) | 0.71193 (19) | 0.0711 (6) |
| H10 | 0.7339 | 0.1989 | 0.7524 | 0.085* |
| C11 | 0.74047 (11) | 0.2948 (2) | 0.62107 (19) | 0.0660 (6) |
| H11 | 0.6928 | 0.2713 | 0.5995 | 0.079* |
| C12 | 0.78589 (9) | 0.37442 (19) | 0.56092 (16) | 0.0537 (4) |
| H12 | 0.7685 | 0.4059 | 0.4996 | 0.064* |
| C13 | 0.90382 (10) | 0.48460 (16) | 0.39035 (14) | 0.0428 (3) |

| | | | | |
|-----|--------------|-------------|---------------|--------------|
| C14 | 0.91498 (10) | 0.5907 (2) | 0.32243 (14) | 0.0507 (4) |
| H14 | 0.9251 | 0.6784 | 0.3456 | 0.061* |
| C15 | 0.91117 (12) | 0.5664 (3) | 0.22073 (16) | 0.0654 (5) |
| H15 | 0.9192 | 0.6376 | 0.1758 | 0.078* |
| C16 | 0.89552 (13) | 0.4373 (3) | 0.18605 (18) | 0.0725 (6) |
| H16 | 0.8922 | 0.4215 | 0.1177 | 0.087* |
| C17 | 0.88481 (14) | 0.3321 (3) | 0.2517 (2) | 0.0783 (7) |
| H17 | 0.8744 | 0.2450 | 0.2273 | 0.094* |
| C18 | 0.88920 (11) | 0.3529 (2) | 0.35474 (17) | 0.0601 (5) |
| H18 | 0.8825 | 0.2804 | 0.3989 | 0.072* |
| C19 | 0.93324 (11) | 0.8460 (2) | 0.92452 (14) | 0.0555 (4) |
| C20 | 0.94493 (15) | 0.7072 (2) | 0.9444 (2) | 0.0787 (6) |
| H20 | 0.9844 | 0.6807 | 0.9852 | 0.094* |
| C21 | 0.89793 (18) | 0.6079 (3) | 0.9033 (3) | 0.0981 (8) |
| H21 | 0.9064 | 0.5160 | 0.9172 | 0.118* |
| C22 | 0.84039 (17) | 0.6437 (3) | 0.8437 (2) | 0.0908 (8) |
| H22 | 0.8097 | 0.5766 | 0.8166 | 0.109* |
| C23 | 0.82711 (15) | 0.7791 (3) | 0.82299 (19) | 0.0835 (7) |
| H23 | 0.7874 | 0.8035 | 0.7819 | 0.100* |
| C24 | 0.87280 (12) | 0.8799 (2) | 0.86322 (17) | 0.0681 (5) |
| H24 | 0.8630 | 0.9714 | 0.8492 | 0.082* |
| C25 | 1.0000 | 1.0000 | 1.1555 (2) | 0.0497 (6) |
| C26 | 1.06462 (16) | 1.0253 (2) | 1.20891 (19) | 0.0680 (6) |
| H26 | 1.1092 | 1.0408 | 1.1752 | 0.082* |
| C27 | 1.0633 (2) | 1.0278 (3) | 1.3133 (2) | 0.0940 (11) |
| H27 | 1.1066 | 1.0488 | 1.3484 | 0.113* |
| C28 | 1.0000 | 1.0000 | 1.3635 (3) | 0.104 (2) |
| H28 | 1.0000 | 1.0000 | 1.4329 | 0.125* |
| N1 | 1.0000 | 0.5000 | 0.55925 (18) | 0.0477 (5) |
| P1 | 0.91740 (2) | 0.51807 (4) | 0.52080 (3) | 0.03734 (9) |
| Sn1 | 1.0000 | 1.0000 | 0.996036 (19) | 0.04870 (5) |
| Cl1 | 0.88562 (3) | 1.16132 (5) | 0.99969 (5) | 0.07087 (13) |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| C1 | 0.0413 (8) | 0.0429 (7) | 0.0452 (8) | -0.0004 (6) | 0.0109 (6) | -0.0061 (6) |
| C2 | 0.0472 (8) | 0.0522 (8) | 0.0735 (14) | 0.0078 (6) | 0.0013 (9) | -0.0093 (10) |
| C3 | 0.0606 (11) | 0.0593 (11) | 0.0979 (19) | 0.0178 (9) | 0.0169 (11) | -0.0040 (11) |
| C4 | 0.0870 (17) | 0.0482 (10) | 0.1007 (18) | 0.0135 (11) | 0.0296 (14) | -0.0106 (11) |
| C5 | 0.0852 (16) | 0.0531 (12) | 0.105 (2) | -0.0121 (11) | 0.0140 (14) | -0.0259 (12) |
| C6 | 0.0527 (10) | 0.0546 (10) | 0.0760 (13) | -0.0077 (8) | 0.0047 (9) | -0.0150 (9) |
| C7 | 0.0381 (7) | 0.0415 (7) | 0.0513 (9) | -0.0010 (6) | 0.0064 (7) | -0.0023 (7) |
| C8 | 0.0569 (11) | 0.0566 (10) | 0.0490 (10) | -0.0034 (8) | 0.0032 (8) | -0.0030 (8) |
| C9 | 0.0928 (16) | 0.0613 (11) | 0.0491 (10) | -0.0055 (10) | 0.0154 (10) | 0.0016 (9) |
| C10 | 0.0732 (14) | 0.0598 (12) | 0.0802 (15) | -0.0155 (10) | 0.0313 (12) | -0.0049 (10) |
| C11 | 0.0459 (10) | 0.0605 (11) | 0.0914 (16) | -0.0101 (8) | 0.0166 (10) | -0.0056 (11) |
| C12 | 0.0390 (8) | 0.0516 (10) | 0.0703 (12) | -0.0042 (7) | 0.0018 (8) | 0.0020 (8) |

| | | | | | | |
|-----|--------------|--------------|-------------|--------------|--------------|---------------|
| C13 | 0.0355 (7) | 0.0512 (9) | 0.0418 (9) | 0.0077 (6) | -0.0030 (6) | -0.0088 (6) |
| C14 | 0.0497 (9) | 0.0579 (9) | 0.0445 (9) | 0.0199 (7) | -0.0037 (7) | 0.0002 (7) |
| C15 | 0.0618 (11) | 0.0859 (15) | 0.0484 (10) | 0.0300 (11) | -0.0056 (9) | 0.0042 (10) |
| C16 | 0.0651 (13) | 0.1060 (18) | 0.0464 (11) | 0.0206 (13) | -0.0085 (9) | -0.0204 (13) |
| C17 | 0.0743 (14) | 0.0871 (17) | 0.0736 (16) | -0.0019 (12) | 0.0025 (12) | -0.0441 (14) |
| C18 | 0.0597 (11) | 0.0558 (11) | 0.0648 (13) | -0.0010 (8) | 0.0035 (9) | -0.0120 (9) |
| C19 | 0.0593 (11) | 0.0659 (11) | 0.0414 (9) | 0.0071 (8) | 0.0049 (8) | -0.0087 (8) |
| C20 | 0.0872 (16) | 0.0715 (13) | 0.0774 (15) | 0.0129 (12) | -0.0088 (12) | -0.0081 (11) |
| C21 | 0.113 (2) | 0.0713 (16) | 0.110 (2) | -0.0072 (15) | -0.0013 (18) | -0.0146 (16) |
| C22 | 0.0943 (19) | 0.0950 (19) | 0.0831 (18) | -0.0156 (15) | 0.0095 (15) | -0.0308 (14) |
| C23 | 0.0711 (15) | 0.114 (2) | 0.0650 (14) | 0.0008 (14) | -0.0075 (11) | -0.0255 (14) |
| C24 | 0.0700 (13) | 0.0775 (13) | 0.0567 (11) | 0.0032 (10) | -0.0080 (9) | -0.0113 (10) |
| C25 | 0.0626 (16) | 0.0476 (13) | 0.0389 (13) | -0.0052 (10) | 0.000 | 0.000 |
| C26 | 0.0810 (15) | 0.0662 (11) | 0.0568 (13) | -0.0148 (10) | -0.0186 (11) | 0.0072 (9) |
| C27 | 0.152 (3) | 0.0699 (14) | 0.0604 (16) | -0.0191 (16) | -0.0434 (19) | 0.0006 (12) |
| C28 | 0.210 (7) | 0.064 (2) | 0.0396 (17) | -0.012 (2) | 0.000 | 0.000 |
| N1 | 0.0341 (9) | 0.0663 (13) | 0.0427 (11) | 0.0008 (8) | 0.000 | 0.000 |
| P1 | 0.03077 (16) | 0.04225 (16) | 0.0390 (2) | 0.00106 (13) | 0.00104 (13) | -0.00220 (15) |
| Sn1 | 0.04949 (8) | 0.06206 (9) | 0.03456 (7) | 0.00872 (6) | 0.000 | 0.000 |
| Cl1 | 0.0614 (2) | 0.0894 (3) | 0.0618 (3) | 0.0292 (2) | -0.0110 (3) | -0.0201 (3) |

Geometric parameters (Å, °)

| | | | |
|---------|-------------|----------------------|-------------|
| C1—C6 | 1.376 (2) | C16—C17 | 1.367 (4) |
| C1—C2 | 1.394 (2) | C16—H16 | 0.9300 |
| C1—P1 | 1.8049 (16) | C17—C18 | 1.396 (4) |
| C2—C3 | 1.377 (2) | C17—H17 | 0.9300 |
| C2—H2 | 0.9300 | C18—H18 | 0.9300 |
| C3—C4 | 1.364 (4) | C19—C24 | 1.398 (3) |
| C3—H3 | 0.9300 | C19—C20 | 1.398 (3) |
| C4—C5 | 1.365 (4) | C19—Sn1 | 2.1476 (19) |
| C4—H4 | 0.9300 | C20—C21 | 1.397 (4) |
| C5—C6 | 1.391 (3) | C20—H20 | 0.9300 |
| C5—H5 | 0.9300 | C21—C22 | 1.349 (4) |
| C6—H6 | 0.9300 | C21—H21 | 0.9300 |
| C7—C8 | 1.384 (3) | C22—C23 | 1.373 (4) |
| C7—C12 | 1.394 (2) | C22—H22 | 0.9300 |
| C7—P1 | 1.7998 (16) | C23—C24 | 1.389 (3) |
| C8—C9 | 1.389 (3) | C23—H23 | 0.9300 |
| C8—H8 | 0.9300 | C24—H24 | 0.9300 |
| C9—C10 | 1.377 (3) | C25—C26 ⁱ | 1.383 (3) |
| C9—H9 | 0.9300 | C25—C26 | 1.383 (3) |
| C10—C11 | 1.365 (4) | C25—Sn1 | 2.134 (3) |
| C10—H10 | 0.9300 | C26—C27 | 1.397 (4) |
| C11—C12 | 1.384 (3) | C26—H26 | 0.9300 |
| C11—H11 | 0.9300 | C27—C28 | 1.346 (5) |
| C12—H12 | 0.9300 | C27—H27 | 0.9300 |
| C13—C18 | 1.398 (3) | C28—C27 ⁱ | 1.345 (5) |

| | | | |
|-------------|-------------|---------------------------|-------------|
| C13—C14 | 1.393 (3) | C28—H28 | 0.9300 |
| C13—P1 | 1.7929 (19) | N1—P1 ⁱⁱ | 1.5763 (9) |
| C14—C15 | 1.383 (3) | N1—P1 | 1.5763 (9) |
| C14—H14 | 0.9300 | Sn1—C19 ⁱ | 2.1476 (19) |
| C15—C16 | 1.374 (4) | Sn1—Cl1 | 2.5858 (4) |
| C15—H15 | 0.9300 | Sn1—Cl1 ⁱ | 2.5858 (4) |
| C6—C1—C2 | 119.70 (16) | C17—C18—C13 | 118.8 (2) |
| C6—C1—P1 | 120.91 (14) | C17—C18—H18 | 120.6 |
| C2—C1—P1 | 119.39 (12) | C13—C18—H18 | 120.6 |
| C1—C2—C3 | 119.87 (18) | C24—C19—C20 | 117.2 (2) |
| C1—C2—H2 | 120.1 | C24—C19—Sn1 | 121.74 (16) |
| C3—C2—H2 | 120.1 | C20—C19—Sn1 | 120.81 (16) |
| C4—C3—C2 | 120.1 (2) | C21—C20—C19 | 120.6 (3) |
| C4—C3—H3 | 120.0 | C21—C20—H20 | 119.7 |
| C2—C3—H3 | 120.0 | C19—C20—H20 | 119.7 |
| C5—C4—C3 | 120.7 (2) | C22—C21—C20 | 120.8 (3) |
| C5—C4—H4 | 119.7 | C22—C21—H21 | 119.6 |
| C3—C4—H4 | 119.7 | C20—C21—H21 | 119.6 |
| C4—C5—C6 | 120.2 (2) | C23—C22—C21 | 120.1 (3) |
| C4—C5—H5 | 119.9 | C23—C22—H22 | 119.9 |
| C6—C5—H5 | 119.9 | C21—C22—H22 | 119.9 |
| C1—C6—C5 | 119.4 (2) | C22—C23—C24 | 120.2 (3) |
| C1—C6—H6 | 120.3 | C22—C23—H23 | 119.9 |
| C5—C6—H6 | 120.3 | C24—C23—H23 | 119.9 |
| C8—C7—C12 | 119.46 (16) | C19—C24—C23 | 121.0 (2) |
| C8—C7—P1 | 118.89 (13) | C19—C24—H24 | 119.5 |
| C12—C7—P1 | 121.54 (14) | C23—C24—H24 | 119.5 |
| C7—C8—C9 | 120.3 (2) | C26 ⁱ —C25—C26 | 117.7 (3) |
| C7—C8—H8 | 119.8 | C26 ⁱ —C25—Sn1 | 121.14 (16) |
| C9—C8—H8 | 119.8 | C26—C25—Sn1 | 121.14 (16) |
| C8—C9—C10 | 119.4 (2) | C25—C26—C27 | 120.4 (3) |
| C8—C9—H9 | 120.3 | C25—C26—H26 | 119.8 |
| C10—C9—H9 | 120.3 | C27—C26—H26 | 119.8 |
| C11—C10—C9 | 120.91 (19) | C28—C27—C26 | 120.6 (3) |
| C11—C10—H10 | 119.5 | C28—C27—H27 | 119.7 |
| C9—C10—H10 | 119.5 | C26—C27—H27 | 119.7 |
| C10—C11—C12 | 120.3 (2) | C27 ⁱ —C28—C27 | 120.1 (4) |
| C10—C11—H11 | 119.9 | C27 ⁱ —C28—H28 | 119.9 |
| C12—C11—H11 | 119.9 | C27—C28—H28 | 119.9 |
| C11—C12—C7 | 119.66 (19) | P1 ⁱⁱ —N1—P1 | 141.90 (17) |
| C11—C12—H12 | 120.2 | N1—P1—C13 | 115.13 (10) |
| C7—C12—H12 | 120.2 | N1—P1—C7 | 108.34 (8) |
| C18—C13—C14 | 119.33 (18) | C13—P1—C7 | 109.30 (8) |
| C18—C13—P1 | 121.71 (15) | N1—P1—C1 | 111.33 (6) |
| C14—C13—P1 | 118.69 (13) | C13—P1—C1 | 105.72 (8) |
| C15—C14—C13 | 120.5 (2) | C7—P1—C1 | 106.69 (7) |
| C15—C14—H14 | 119.8 | C25—Sn1—C19 ⁱ | 116.46 (5) |

| | | | |
|-------------|-----------|--|-------------|
| C13—C14—H14 | 119.8 | C25—Sn1—C19 | 116.46 (5) |
| C16—C15—C14 | 120.0 (2) | C19 ⁱ —Sn1—C19 | 127.07 (10) |
| C16—C15—H15 | 120.0 | C25—Sn1—Cl1 | 88.916 (18) |
| C14—C15—H15 | 120.0 | C19 ⁱ —Sn1—Cl1 | 91.27 (5) |
| C17—C16—C15 | 120.2 (2) | C19—Sn1—Cl1 | 89.70 (5) |
| C17—C16—H16 | 119.9 | C25—Sn1—Cl1 ⁱ | 88.917 (18) |
| C15—C16—H16 | 119.9 | C19 ⁱ —Sn1—Cl1 ⁱ | 89.70 (5) |
| C16—C17—C18 | 121.2 (2) | C19—Sn1—Cl1 ⁱ | 91.27 (5) |
| C16—C17—H17 | 119.4 | Cl1—Sn1—Cl1 ⁱ | 177.83 (4) |
| C18—C17—H17 | 119.4 | | |

Symmetry codes: (i) $-x+2, -y+2, z$; (ii) $-x+2, -y+1, z$.

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-----------------------------------|-------|-------------|-------------|---------------|
| C9—H9 \cdots Cl1 ⁱⁱⁱ | 0.93 | 2.79 | 3.718 (2) | 173 |

Symmetry code: (iii) $x, y-1, z$.