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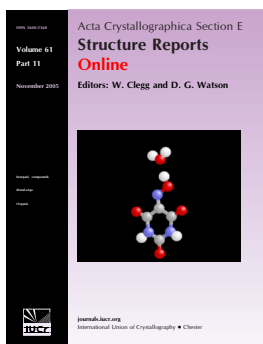
Editors: W. T. A. Harrison, H. Stoeckli-Evans,  
E. R. T. Tiekink and M. Weil

## Dicyclohexylammonium trimethylbis(hydrogen phenylphosphonato)stannate(IV)

Tidiane Diop, Libasse Diop, Cheikh A. K. Diop, Kieran C. Molloy and Gabriele Kociok-Köhn

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## Dicyclohexylammonium trimethylbis-(hydrogen phenylphosphonato)-stannate(IV)

Tidiane Diop,<sup>a</sup> Libasse Diop,<sup>a\*</sup> Cheikh A. K. Diop,<sup>a</sup>  
Kieran C. Molloy<sup>b</sup> and Gabriele Kociok-Köhn<sup>b</sup>

<sup>a</sup>Laboratoire de Chimie Minérale et Analytique, Département de Chimie, Faculté des Sciences et Techniques, Université Cheikh Anta Diop, Dakar, Senegal, and

<sup>b</sup>Department of Chemistry, University of Bath, Claverton Down, Bath BA2 7AY, England

Correspondence e-mail: dlibasse@gmail.com

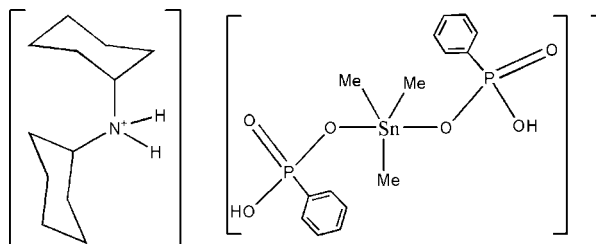
Received 28 October 2011; accepted 20 November 2011

Key indicators: single-crystal X-ray study;  $T = 150$  K; mean  $\sigma(C-C) = 0.007$  Å;  $R$  factor = 0.047;  $wR$  factor = 0.124; data-to-parameter ratio = 20.4.

In the title compound,  $(C_{12}H_{24}N)[Sn(CH_3)_3(C_6H_6O_3P)_2]$ , the  $SnMe_3$  residues are axially coordinated by two monodentate  $[PhPO_3H]^-$  anions, leading to a trigonal-bipyramidal geometry for the  $Sn^{IV}$  atom. The two  $[SnMe_3(PhPO_3H)_2]^-$  anions in the unit cell are associated into infinite chains along the  $a$  axis by  $O-H\cdots O$  hydrogen bonds involving the hydroxy group of the hydrogen phenylphosphonate ion. The chains interact with one another *via*  $O-H\cdots O$  hydrogen bonds along the  $c$  axis. These networks of anions assemble with the dicyclohexylammonium ion through  $N-H\cdots O$  hydrogen bonds, forming a three-dimensional network.

### Related literature

For related organotin derivatives, see: Weakley (1976); Molloy *et al.* (1981); Evans & Karpel (1985); Gielen *et al.* (1995); Yin & Wang (2004); Kapoor *et al.* (2005); Zhang *et al.* (2006). For our recent work on the coordination ability of oxyanions, see: Diop *et al.* (2002, 2003); Diallo *et al.* (2009).



### Experimental

#### Crystal data

$(C_{12}H_{24}N)[Sn(CH_3)_3(C_6H_6O_3P)_2]$   
 $M_r = 660.27$

Triclinic,  $P\bar{1}$   
 $a = 10.8718$  (5) Å

$b = 12.7103$  (7) Å  
 $c = 13.3218$  (7) Å  
 $\alpha = 100.625$  (3)°  
 $\beta = 103.687$  (3)°  
 $\gamma = 111.996$  (3)°  
 $V = 1580.41$  (14) Å<sup>3</sup>

$Z = 2$   
Mo  $K\alpha$  radiation  
 $\mu = 0.95$  mm<sup>-1</sup>  
 $T = 150$  K  
 $0.45 \times 0.30 \times 0.20$  mm

#### Data collection

Nonius KappaCCD diffractometer  
Absorption correction: multi-scan  
(*SORTAV*; Blessing, 1995)  
 $T_{min} = 0.675$ ,  $T_{max} = 0.833$

21070 measured reflections  
7212 independent reflections  
6014 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.068$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$   
 $wR(F^2) = 0.124$   
 $S = 1.09$   
7212 reflections  
353 parameters  
2 restraints

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{max} = 1.86$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -1.80$  e Å<sup>-3</sup>

**Table 1**

Selected bond lengths (Å).

Sn—C1	2.132 (4)	Sn—O1	2.227 (2)
Sn—C2	2.114 (4)	Sn—O4	2.241 (3)
Sn—C3	2.134 (4)		

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O2-H2\cdots O6^i$	0.76 (4)	1.88 (4)	2.642 (4)	178 (7)
$O5-H5A\cdots O6^{ii}$	0.94 (7)	1.67 (7)	2.596 (4)	169 (6)
$N-H10A\cdots O3$	0.89 (2)	1.92 (2)	2.798 (4)	169 (4)
$N-H10B\cdots O3^{iii}$	0.95 (4)	1.83 (4)	2.759 (4)	165 (4)

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

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: VN2021).

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**supplementary materials**

*Acta Cryst.* (2011). E67, m1872-m1873 [doi:10.1107/S1600536811049567]v

## Dicyclohexylammonium trimethylbis(hydrogen phenylphosphonato)stannate(IV)t

T. Diop, L. Diop, C. A. K. Diop, K. C. Molloy and G. Kociok-Köhnt

### Comment

Research on organotin derivatives has been an attractive area because of their numerous applications and their versatile structure (Evans & Karpel, 1985; Kapoor *et al.*, 2005; Zhang *et al.*, 2006; Yin & Wang, 2004; Gielen *et al.*, 1995). In the scope of our research work on the coordination ability of oxyanions (Diop *et al.*, 2002, Diallo *et al.*, 2009; Diop *et al.*, 2003) and our interest to synthesize new organotin derivatives for biological tests, we elucidate here the structure of the title compound, [C<sub>15</sub>H<sub>21</sub>O<sub>6</sub>P<sub>2</sub>Sn, C<sub>12</sub>H<sub>24</sub>N] (Fig. 1).v

The crystal structure of the molecule is shown in Fig 2: hydrogen bonds between pairs of [SnMe<sub>3</sub>(PhPO<sub>3</sub>H)<sub>2</sub>]<sup>-</sup> generate a six membered ring, comprise a honey comb network by virtue of the hydrogen bonds between the ligands as in *catena*-trimethyltin(IV)phenylarsenate, reported by Diop *et al.* (2002).v

Each SnMe<sub>3</sub> unit is σ bonded to two [PhPO<sub>3</sub>H]<sup>-</sup> via one negatively charged oxygen atom, leading to a *trans* trigonal bipyramidal environment around the tin centre (Fig. 1). The resulting anions [SnMe<sub>3</sub>(PhPO<sub>3</sub>H)<sub>2</sub>]<sup>-</sup> are associated through hydrogen bonds OH...O, along the *b* axis into pairs and along the *a* axis to form infinite layers (Fig. 2). The different layers are connected by NH...O hydrogen bonds along the *b* axis. The hydrogen bonds render the P=O and P—O bond distances almost equal (P(1)—O(3) 1.506 (3) Å, P(1)—O(1): 1.509 (2) Å, P(1)—O(2): 1.569 (3) Å) while different of those in the parent phenylphosphonic acid PhPO<sub>3</sub>H<sub>2</sub> (Weakley, 1976) (1.496 Å for P=O and 1.545 Å for P—OH). The geometry around the phosphorous atom in the ligands is a distorted tetrahedron (O(3)—P(1)—O(1): 115.48°(15), O(1)—P(1)—C(4): 107.03°(15)) owing to steric hindrance. The sum of the C—Sn—C angle is 59.99° and the O(1)—Sn—O(4) angle of 178.24°(9) indicate a nearly perfect *trans* trigonal bipyramidal arrangement with the carbon atoms of the methyl occupying the equatorial positions while the oxygen atoms are on the apical positions. The two Sn—O distances observed here - Sn—O(1) 2.227 (2) Å; Sn—O(4) 2.240 (3) Å - are shorter than the distances reported for (α-phenylphosphonato)trimethyltin(IV) by Molloy *et al.* (1981) (2.240 (6) Å and 2.319 (5) Å).v

### Experimental

Cy<sub>2</sub>NH<sub>2</sub>PhPO<sub>3</sub>H (*L*) is obtained on mixing dicyclohexylamine with PhPO<sub>3</sub>H<sub>2</sub> in water in 1/1 ratio. The title compound has been obtained as white crystalline solid by reacting (*L*) with trimethyltinchloride in ethanol (2/1 ratio *M*, p:170°). Slow solvent evaporation of the solution afforded colorless crystals suitable for x-ray structure determination. All the chemicals (Aldrich) were used without any further purification.v

### Refinement

All C-bound H-atoms were positioned geometrically and were included in the refinement in the riding model approximation, with U<sub>iso</sub>(H) set to 1.2 and 1.5 U<sub>eq</sub>(C). All N- and O-bound H-atoms have been located in the difference Fourier map

# supplementary materials

and were refined freely. However, H(2) binding to O(2) and H(10A) binding to N had to be restrained with O—H = 0.82 (2) Å and N—H = 0.87 (2) Å.

## Figures

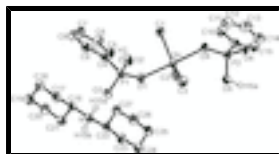


Fig. 1. : The molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

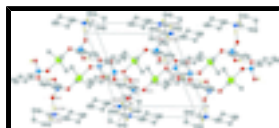


Fig. 2. : Three dimensional structure showing the hydrogen bonds as dotted lines.

## Dicyclohexylammonium bis(hydrogen phenylphosphonato)trimethylstannate(IV)

### Crystal data

(C<sub>12</sub>H<sub>24</sub>N)[Sn(CH<sub>3</sub>)<sub>3</sub>(C<sub>6</sub>H<sub>6</sub>O<sub>3</sub>P)<sub>2</sub>]

*M<sub>r</sub>* = 660.27

Triclinic, *P* $\bar{1}$

Hall symbol: -*P* 1

*a* = 10.8718 (5) Å

*b* = 12.7103 (7) Å

*c* = 13.3218 (7) Å

$\alpha$  = 100.625 (3)°

$\beta$  = 103.687 (3)°

$\gamma$  = 111.996 (3)°

*V* = 1580.41 (14) Å<sup>3</sup>

*Z* = 2

*F*(000) = 684

*D<sub>x</sub>* = 1.387 Mg m<sup>-3</sup>

Mo *K* $\alpha$  radiation,  $\lambda$  = 0.71073 Å

Cell parameters from 47204 reflections

$\theta$  = 2.9–27.5°

$\mu$  = 0.95 mm<sup>-1</sup>

*T* = 150 K

Plate, colourless

0.45 × 0.30 × 0.20 mm

### Data collection

Nonius KappaCCD  
diffractometer

Radiation source: fine-focus sealed tube  
graphite

166 2.0 degree images with  $\omega$  scans

Absorption correction: multi-scan  
(*SORTAV*; Blessing, 1995)

*T<sub>min</sub>* = 0.675, *T<sub>max</sub>* = 0.833

21070 measured reflections

7212 independent reflections

6014 reflections with *I* > 2 $\sigma$ (*I*)

*R<sub>int</sub>* = 0.068

$\theta_{\text{max}}$  = 27.5°,  $\theta_{\text{min}}$  = 3.8°

*h* = -14→14

*k* = -16→16

*l* = -17→16

### Refinement

Refinement on *F*<sup>2</sup>

Least-squares matrix: full

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$[F^2 > 2\sigma(F^2)] = 0.047v$	Hydrogen site location: inferred from neighbouring sitesv
$wR(F^2) = 0.124v$	H atoms treated by a mixture of independent and constrained refinementv
$S = 1.09v$	$w = 1/[\sigma^2(F_o^2) + (0.0655P)^2 + 1.1841P]$
7212 reflectionsv	where $P = (F_o^2 + 2F_c^2)/3v$
353 parametersv	$(\Delta/\sigma)_{\max} < 0.001v$
2 restraintsv	$\Delta\rho_{\max} = 1.86 \text{ e } \text{\AA}^{-3}v$
	$\Delta\rho_{\min} = -1.80 \text{ e } \text{\AA}^{-3}v$

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.v

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $v$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $v$ -factors  $v$  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  $v$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $v$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $v$ -factors based on ALL data will be even larger.v

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eqv}}$
Snv	0.39323 (2)v	0.58948 (2)v	0.341865 (19)v	0.02776 (9)v
P1v	0.74338 (9)v	0.72317 (8)v	0.37030 (7)v	0.02711 (19)v
P2v	0.06261 (9)v	0.44906 (8)v	0.36638 (8)v	0.02827 (19)v
O1v	0.6010 (2)v	0.7236 (2)v	0.3496 (2)v	0.0320 (5)v
O2v	0.7419 (3)v	0.6228 (2)v	0.4238 (2)v	0.0353 (6)v
H2v	0.807 (5)v	0.623 (5)v	0.462 (4)v	0.070 (18)*v
O3v	0.8675 (2)v	0.8403 (2)v	0.4370 (2)v	0.0310 (5)v
O4v	0.1834 (3)v	0.4514 (2)v	0.3290 (2)v	0.0360 (6)v
O5v	0.0892 (3)v	0.5817 (2)v	0.4150 (2)v	0.0338 (6)v
H5Av	0.039 (7)v	0.585 (6)v	0.463 (5)v	0.08 (2)*v
O6v	0.0351 (2)v	0.3812 (2)v	0.4473 (2)v	0.0306 (5)v
Nv	0.9314 (3)v	1.0380 (3)v	0.3600 (2)v	0.0291 (6)v
H10Av	0.906 (5)v	0.970 (3)v	0.376 (4)v	0.043 (12)*v
H10Bv	1.004 (4)v	1.092 (4)v	0.426 (3)v	0.029 (10)*v
C1v	0.4197 (4)v	0.4478 (4)v	0.2508 (3)v	0.0357 (8)v
H1Av	0.3304v	0.3754v	0.2223v	0.053*v
H1Bv	0.4921v	0.4334v	0.2977v	0.053*v
H1Cv	0.4488v	0.4694v	0.1904v	0.053*v
C2v	0.4641 (4)v	0.6421 (4)v	0.5132 (3)v	0.0373 (8)v
H2Av	0.5502v	0.6326v	0.5399v	0.056*v
H2Bv	0.3912v	0.5924v	0.5378v	0.056*v
H2Cv	0.4837v	0.7257v	0.5412v	0.056*v
C3v	0.2929 (4)v	0.6733 (4)v	0.2497 (3)v	0.0396 (9)v



## supplementary materials

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H3Av	0.2375v	0.6994v	0.2876v	0.059*v
H3Bv	0.2307v	0.6166v	0.1782v	0.059*v
H3Cv	0.3646v	0.7424v	0.2409v	0.059*v
C4v	0.7614 (4)v	0.6798 (3)v	0.2399 (3)v	0.0297 (7)v
C5v	0.6643 (4)v	0.6721 (4)v	0.1461 (3)v	0.0433 (10)v
H5v	0.5856v	0.6861v	0.1506v	0.052*v
C6v	0.6811 (6)v	0.6443 (6)v	0.0462 (4)v	0.0610 (14)v
H6v	0.6148v	0.6405v	-0.0170v	0.073*v
C7v	0.7947 (5)v	0.6219 (5)v	0.0383 (3)v	0.0516 (11)v
H7v	0.8058v	0.6026v	-0.0304v	0.062*v
C8v	0.8919 (5)v	0.6278 (4)v	0.1304 (4)v	0.0430 (9)v
H8v	0.9689v	0.6115v	0.1252v	0.052*v
C9v	0.8754 (4)v	0.6579 (3)v	0.2309 (3)v	0.0355 (8)v
H9v	0.9430v	0.6635v	0.2942v	0.043*v
C10v	-0.0932 (4)v	0.3826 (3)v	0.2475 (3)v	0.0322 (7)v
C11v	-0.0850 (5)v	0.3461 (4)v	0.1446 (3)v	0.0444 (10)v
H11v	0.0032v	0.3562v	0.1372v	0.053*v
C12v	-0.2058 (6)v	0.2946 (5)v	0.0527 (4)v	0.0562 (12)v
H12v	-0.2001v	0.2691v	-0.0170v	0.067*v
C13v	-0.3337 (6)v	0.2812 (5)v	0.0639 (4)v	0.0595 (13)v
H13v	-0.4159v	0.2462v	0.0014v	0.071*v
C14v	-0.3430 (5)v	0.3180 (4)v	0.1645 (4)v	0.0512 (11)v
H14v	-0.4314v	0.3085v	0.1711v	0.061*v
C15v	-0.2241 (4)v	0.3688 (4)v	0.2559 (3)v	0.0391 (9)v
H15v	-0.2312v	0.3946v	0.3250v	0.047*v
C16v	0.9824 (4)v	1.0236 (3)v	0.2651 (3)v	0.0314 (7)v
H16v	0.9017v	0.9615v	0.2010v	0.038*v
C17v	1.0365 (5)v	1.1398 (4)v	0.2371 (3)v	0.0406 (9)v
H17Av	1.1137v	1.2033v	0.3008v	0.049*v
H17Bv	0.9597v	1.1641v	0.2179v	0.049*v
C18v	1.0900 (5)v	1.1238 (4)v	0.1419 (4)v	0.0465 (10)v
H18Av	1.1312v	1.2012v	0.1279v	0.056*v
H18Bv	1.0099v	1.0674v	0.0761v	0.056*v
C19v	1.2011 (5)v	1.0767 (4)v	0.1639 (4)v	0.0470 (10)v
H19Av	1.2276v	1.0617v	0.0984v	0.056*v
H19Bv	1.2864v	1.1377v	0.2237v	0.056*v
C20v	1.1468 (4)v	0.9626 (4)v	0.1941 (4)v	0.0438 (9)v
H20Av	1.2227v	0.9371v	0.2122v	0.053*v
H20Bv	1.0678v	0.8990v	0.1315v	0.053*v
C21v	1.0967 (4)v	0.9810 (4)v	0.2915 (3)v	0.0376 (8)v
H21Av	1.0590v	0.9053v	0.3089v	0.045*v
H21Bv	1.1770v	1.0408v	0.3557v	0.045*v
C22v	0.8128 (4)v	1.0751 (3)v	0.3484 (3)v	0.0325 (8)v
H22v	0.8446v	1.1542v	0.3349v	0.039*v
C23v	0.7833 (4)v	1.0885 (4)v	0.4551 (3)v	0.0395 (9)v
H23Av	0.7567v	1.0119v	0.4717v	0.047*v
H23Bv	0.8695v	1.1491v	0.5144v	0.047*v
C24v	0.6648 (4)v	1.1259 (4)v	0.4481 (4)v	0.0472 (10)v
H24Av	0.6941v	1.2052v	0.4367v	0.057*v

H24Bv	0.6447v	1.1319v	0.5171v	0.057*v
C25v	0.5317 (4)v	1.0355 (4)v	0.3547 (4)v	0.0499 (11)v
H25Av	0.4982v	0.9577v	0.3690v	0.060*v
H25Bv	0.4568v	1.0626v	0.3497v	0.060*v
C26v	0.5605 (4)v	1.0211 (4)v	0.2482 (4)v	0.0493 (11)v
H26Av	0.5843v	1.0969v	0.2302v	0.059*v
H26Bv	0.4745v	0.9591v	0.1897v	0.059*v
C27v	0.6824 (4)v	0.9860 (4)v	0.2541 (3)v	0.0377 (8)v
H27Av	0.6544v	0.9057v	0.2632v	0.045*v
H27Bv	0.7035v	0.9833v	0.1856v	0.045*v

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11v}$	$U^{22v}$	$U^{33v}$	$U^{12v}$	$U^{13v}$	$U^{23v}$
Snv	0.02108 (13)v	0.03255 (14)v	0.03159 (14)v	0.01278 (10)v	0.00933 (9)v	0.01115 (9)v
P1v	0.0195 (4)v	0.0280 (4)v	0.0322 (4)v	0.0092 (4)v	0.0066 (3)v	0.0106 (3)v
P2v	0.0206 (4)v	0.0297 (5)v	0.0366 (5)v	0.0116 (4)v	0.0107 (3)v	0.0121 (4)v
O1v	0.0219 (12)v	0.0349 (13)v	0.0415 (14)v	0.0131 (11)v	0.0104 (10)v	0.0156 (11)v
O2v	0.0234 (13)v	0.0372 (14)v	0.0439 (15)v	0.0105 (11)v	0.0067 (11)v	0.0213 (12)v
O3v	0.0209 (11)v	0.0320 (13)v	0.0333 (13)v	0.0073 (10)v	0.0059 (9)v	0.0086 (10)v
O4v	0.0254 (12)v	0.0364 (14)v	0.0504 (16)v	0.0141 (11)v	0.0181 (11)v	0.0146 (12)v
O5v	0.0296 (13)v	0.0310 (13)v	0.0426 (14)v	0.0128 (11)v	0.0144 (11)v	0.0134 (11)v
O6v	0.0243 (12)v	0.0317 (13)v	0.0379 (13)v	0.0132 (11)v	0.0100 (10)v	0.0138 (10)v
Nv	0.0240 (14)v	0.0287 (16)v	0.0314 (15)v	0.0098 (13)v	0.0065 (12)v	0.0097 (12)v
C1v	0.0299 (18)v	0.041 (2)v	0.039 (2)v	0.0182 (17)v	0.0129 (15)v	0.0108 (16)v
C2v	0.038 (2)v	0.045 (2)v	0.038 (2)v	0.0237 (18)v	0.0148 (16)v	0.0166 (17)v
C3v	0.0293 (18)v	0.045 (2)v	0.048 (2)v	0.0175 (17)v	0.0108 (16)v	0.0216 (18)v
C4v	0.0246 (16)v	0.0316 (18)v	0.0337 (18)v	0.0129 (15)v	0.0089 (13)v	0.0116 (14)v
C5v	0.034 (2)v	0.061 (3)v	0.037 (2)v	0.028 (2)v	0.0082 (16)v	0.0097 (18)v
C6v	0.054 (3)v	0.100 (4)v	0.036 (2)v	0.048 (3)v	0.008 (2)v	0.013 (2)v
C7v	0.057 (3)v	0.074 (3)v	0.034 (2)v	0.036 (3)v	0.0198 (19)v	0.014 (2)v
C8v	0.042 (2)v	0.049 (2)v	0.049 (2)v	0.029 (2)v	0.0184 (18)v	0.0150 (19)v
C9v	0.0273 (18)v	0.039 (2)v	0.041 (2)v	0.0154 (16)v	0.0094 (15)v	0.0140 (16)v
C10v	0.0314 (18)v	0.0330 (19)v	0.0383 (19)v	0.0183 (16)v	0.0124 (15)v	0.0146 (15)v
C11v	0.047 (2)v	0.054 (3)v	0.042 (2)v	0.029 (2)v	0.0163 (18)v	0.0181 (19)v
C12v	0.064 (3)v	0.067 (3)v	0.039 (2)v	0.037 (3)v	0.009 (2)v	0.014 (2)v
C13v	0.053 (3)v	0.059 (3)v	0.050 (3)v	0.030 (3)v	-0.009 (2)v	0.005 (2)v
C14v	0.031 (2)v	0.051 (3)v	0.063 (3)v	0.021 (2)v	0.0031 (19)v	0.009 (2)v
C15v	0.0289 (18)v	0.042 (2)v	0.045 (2)v	0.0182 (17)v	0.0095 (16)v	0.0103 (17)v
C16v	0.0270 (17)v	0.0316 (18)v	0.0313 (17)v	0.0097 (15)v	0.0087 (14)v	0.0080 (14)v
C17v	0.047 (2)v	0.036 (2)v	0.044 (2)v	0.0195 (19)v	0.0187 (18)v	0.0167 (17)v
C18v	0.055 (3)v	0.046 (2)v	0.044 (2)v	0.021 (2)v	0.025 (2)v	0.0191 (19)v
C19v	0.039 (2)v	0.052 (3)v	0.049 (2)v	0.016 (2)v	0.0211 (19)v	0.015 (2)v
C20v	0.035 (2)v	0.046 (2)v	0.050 (2)v	0.0188 (19)v	0.0157 (18)v	0.0097 (19)v
C21v	0.0325 (19)v	0.038 (2)v	0.043 (2)v	0.0164 (17)v	0.0136 (16)v	0.0127 (16)v
C22v	0.0248 (17)v	0.0293 (18)v	0.042 (2)v	0.0122 (15)v	0.0079 (14)v	0.0116 (15)v
C23v	0.0301 (19)v	0.044 (2)v	0.042 (2)v	0.0158 (17)v	0.0132 (16)v	0.0075 (17)v
C24v	0.033 (2)v	0.047 (2)v	0.058 (3)v	0.0178 (19)v	0.0167 (19)v	0.006 (2)v

## supplementary materials

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C25v	0.0269 (19)v	0.044 (2)v	0.071 (3)v	0.0136 (18)v	0.0155 (19)v	0.005 (2)v
C26v	0.029 (2)v	0.049 (3)v	0.058 (3)v	0.0165 (19)v	0.0013 (18)v	0.008 (2)v
C27v	0.0280 (18)v	0.041 (2)v	0.040 (2)v	0.0156 (17)v	0.0054 (15)v	0.0096 (16)v

### *Geometric parameters (Å, °)*

Sn—C1v	2.132 (4)v	C11—H11v	0.9500v
Sn—C2v	2.114 (4)v	C12—C13v	1.383 (8)v
Sn—C3v	2.134 (4)v	C12—H12v	0.9500v
Sn—O1v	2.227 (2)v	C13—C14v	1.376 (7)v
Sn—O4v	2.241 (3)v	C13—H13v	0.9500v
P1—O3v	1.506 (3)v	C14—C15v	1.383 (6)v
P1—O1v	1.509 (2)v	C14—H14v	0.9500v
P1—O2v	1.569 (3)v	C15—H15v	0.9500v
P1—C4v	1.803 (4)v	C16—C17v	1.524 (5)v
P2—O4v	1.503 (3)v	C16—C21v	1.525 (5)v
P2—O6v	1.516 (3)v	C16—H16v	1.0000v
P2—O5v	1.578 (3)v	C17—C18v	1.527 (6)v
P2—C10v	1.805 (4)v	C17—H17Av	0.9900v
O2—H2v	0.76 (4)v	C17—H17Bv	0.9900v
O5—H5Av	0.94 (7)v	C18—C19v	1.529 (6)v
N—C16v	1.503 (5)v	C18—H18Av	0.9900v
N—C22v	1.515 (5)v	C18—H18Bv	0.9900v
N—H10Av	0.887 (19)v	C19—C20v	1.517 (6)v
N—H10Bv	0.95 (4)v	C19—H19Av	0.9900v
C1—H1Av	0.9800v	C19—H19Bv	0.9900v
C1—H1Bv	0.9800v	C20—C21v	1.534 (6)v
C1—H1Cv	0.9800v	C20—H20Av	0.9900v
C2—H2Av	0.9800v	C20—H20Bv	0.9900v
C2—H2Bv	0.9800v	C21—H21Av	0.9900v
C2—H2Cv	0.9800v	C21—H21Bv	0.9900v
C3—H3Av	0.9800v	C22—C27v	1.517 (5)v
C3—H3Bv	0.9800v	C22—C23v	1.522 (5)v
C3—H3Cv	0.9800v	C22—H22v	1.0000v
C4—C5v	1.393 (5)v	C23—C24v	1.521 (5)v
C4—C9v	1.395 (5)v	C23—H23Av	0.9900v
C5—C6v	1.385 (6)v	C23—H23Bv	0.9900v
C5—H5v	0.9500v	C24—C25v	1.528 (6)v
C6—C7v	1.390 (7)v	C24—H24Av	0.9900v
C6—H6v	0.9500v	C24—H24Bv	0.9900v
C7—C8v	1.386 (6)v	C25—C26v	1.517 (7)v
C7—H7v	0.9500v	C25—H25Av	0.9900v
C8—C9v	1.395 (6)v	C25—H25Bv	0.9900v
C8—H8v	0.9500v	C26—C27v	1.539 (6)v
C9—H9v	0.9500v	C26—H26Av	0.9900v
C10—C11v	1.399 (5)v	C26—H26Bv	0.9900v
C10—C15v	1.401 (5)v	C27—H27Av	0.9900v
C11—C12v	1.398 (6)v	C27—H27Bv	0.9900v
C2—Sn—C1v	121.15 (15)v	C12—C13—H13v	119.7v

C2—Sn—C3v	122.89 (16)v	C13—C14—C15v	120.1 (4)v
C1—Sn—C3v	115.97 (16)v	C13—C14—H14v	119.9v
C2—Sn—O1v	88.92 (13)v	C15—C14—H14v	119.9v
C1—Sn—O1v	91.77 (12)v	C14—C15—C10v	120.6 (4)v
C3—Sn—O1v	89.14 (13)v	C14—C15—H15v	119.7v
C2—Sn—O4v	92.68 (13)v	C10—C15—H15v	119.7v
C1—Sn—O4v	86.78 (13)v	N—C16—C17v	110.9 (3)v
C3—Sn—O4v	90.59 (13)v	N—C16—C21v	109.1 (3)v
O1—Sn—O4v	178.24 (9)v	C17—C16—C21v	111.2 (3)v
O3—P1—O1v	115.48 (15)v	N—C16—H16v	108.5v
O3—P1—O2v	110.97 (15)v	C17—C16—H16v	108.5v
O1—P1—O2v	107.81 (15)v	C21—C16—H16v	108.5v
O3—P1—C4v	108.23 (15)v	C16—C17—C18v	110.1 (3)v
O1—P1—C4v	107.03 (15)v	C16—C17—H17Av	109.6v
O2—P1—C4v	106.94 (16)v	C18—C17—H17Av	109.6v
O4—P2—O6v	115.57 (15)v	C16—C17—H17Bv	109.6v
O4—P2—O5v	108.23 (15)v	C18—C17—H17Bv	109.6v
O6—P2—O5v	110.03 (15)v	H17A—C17—H17Bv	108.2v
O4—P2—C10v	107.22 (17)v	C17—C18—C19v	111.8 (4)v
O6—P2—C10v	108.73 (16)v	C17—C18—H18Av	109.3v
O5—P2—C10v	106.67 (16)v	C19—C18—H18Av	109.3v
P1—O1—Snv	132.28 (15)v	C17—C18—H18Bv	109.3v
P1—O2—H2v	125 (5)v	C19—C18—H18Bv	109.3v
P2—O4—Snv	136.69 (16)v	H18A—C18—H18Bv	107.9v
P2—O5—H5Av	110 (4)v	C20—C19—C18v	111.4 (4)v
C16—N—C22v	117.5 (3)v	C20—C19—H19Av	109.3v
C16—N—H10Av	107 (3)v	C18—C19—H19Av	109.3v
C22—N—H10Av	109 (3)v	C20—C19—H19Bv	109.3v
C16—N—H10Bv	114 (2)v	C18—C19—H19Bv	109.3v
C22—N—H10Bv	106 (2)v	H19A—C19—H19Bv	108.0v
H10A—N—H10Bv	102 (4)v	C19—C20—C21v	110.7 (3)v
Sn—C1—H1Av	109.5v	C19—C20—H20Av	109.5v
Sn—C1—H1Bv	109.5v	C21—C20—H20Av	109.5v
H1A—C1—H1Bv	109.5v	C19—C20—H20Bv	109.5v
Sn—C1—H1Cv	109.5v	C21—C20—H20Bv	109.5v
H1A—C1—H1Cv	109.5v	H20A—C20—H20Bv	108.1v
H1B—C1—H1Cv	109.5v	C16—C21—C20v	109.7 (3)v
Sn—C2—H2Av	109.5v	C16—C21—H21Av	109.7v
Sn—C2—H2Bv	109.5v	C20—C21—H21Av	109.7v
H2A—C2—H2Bv	109.5v	C16—C21—H21Bv	109.7v
Sn—C2—H2Cv	109.5v	C20—C21—H21Bv	109.7v
H2A—C2—H2Cv	109.5v	H21A—C21—H21Bv	108.2v
H2B—C2—H2Cv	109.5v	N—C22—C27v	111.3 (3)v
Sn—C3—H3Av	109.5v	N—C22—C23v	108.1 (3)v
Sn—C3—H3Bv	109.5v	C27—C22—C23v	111.6 (3)v
H3A—C3—H3Bv	109.5v	N—C22—H22v	108.6v
Sn—C3—H3Cv	109.5v	C27—C22—H22v	108.6v
H3A—C3—H3Cv	109.5v	C23—C22—H22v	108.6v
H3B—C3—H3Cv	109.5v	C24—C23—C22v	110.4 (3)v

## supplementary materials

C5—C4—C9v	118.5 (3)v	C24—C23—H23Av	109.6v
C5—C4—P1v	120.5 (3)v	C22—C23—H23Av	109.6v
C9—C4—P1v	121.0 (3)v	C24—C23—H23Bv	109.6v
C6—C5—C4v	120.8 (4)v	C22—C23—H23Bv	109.6v
C6—C5—H5v	119.6v	H23A—C23—H23Bv	108.1v
C4—C5—H5v	119.6v	C23—C24—C25v	110.5 (4)v
C5—C6—C7v	120.1 (4)v	C23—C24—H24Av	109.5v
C5—C6—H6v	119.9v	C25—C24—H24Av	109.5v
C7—C6—H6v	119.9v	C23—C24—H24Bv	109.5v
C8—C7—C6v	120.1 (4)v	C25—C24—H24Bv	109.5v
C8—C7—H7v	120.0v	H24A—C24—H24Bv	108.1v
C6—C7—H7v	120.0v	C26—C25—C24v	110.8 (4)v
C7—C8—C9v	119.4 (4)v	C26—C25—H25Av	109.5v
C7—C8—H8v	120.3v	C24—C25—H25Av	109.5v
C9—C8—H8v	120.3v	C26—C25—H25Bv	109.5v
C8—C9—C4v	121.1 (4)v	C24—C25—H25Bv	109.5v
C8—C9—H9v	119.4v	H25A—C25—H25Bv	108.1v
C4—C9—H9v	119.4v	C25—C26—C27v	111.4 (4)v
C11—C10—C15v	118.6 (4)v	C25—C26—H26Av	109.3v
C11—C10—P2v	120.5 (3)v	C27—C26—H26Av	109.3v
C15—C10—P2v	120.9 (3)v	C25—C26—H26Bv	109.3v
C12—C11—C10v	120.3 (4)v	C27—C26—H26Bv	109.3v
C12—C11—H11v	119.8v	H26A—C26—H26Bv	108.0v
C10—C11—H11v	119.8v	C22—C27—C26v	110.4 (3)v
C13—C12—C11v	119.6 (5)v	C22—C27—H27Av	109.6v
C13—C12—H12v	120.2v	C26—C27—H27Av	109.6v
C11—C12—H12v	120.2v	C22—C27—H27Bv	109.6v
C14—C13—C12v	120.7 (4)v	C26—C27—H27Bv	109.6v
C14—C13—H13v	119.7v	H27A—C27—H27Bv	108.1v

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-Hv$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2—H2 $\cdots$ O6 <sup>iv</sup>	0.76 (4)v	1.88 (4)v	2.642 (4)v	178 (7)v
O5—H5A $\cdots$ O6 <sup>iiiv</sup>	0.94 (7)v	1.67 (7)v	2.596 (4)v	169 (6)v
N—H10A $\cdots$ O3v	0.89 (2)v	1.92 (2)v	2.798 (4)v	169 (4)v
N—H10B $\cdots$ O3 <sup>iiiv</sup>	0.95 (4)v	1.83 (4)v	2.759 (4)v	165 (4)v

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

Fig. 1m

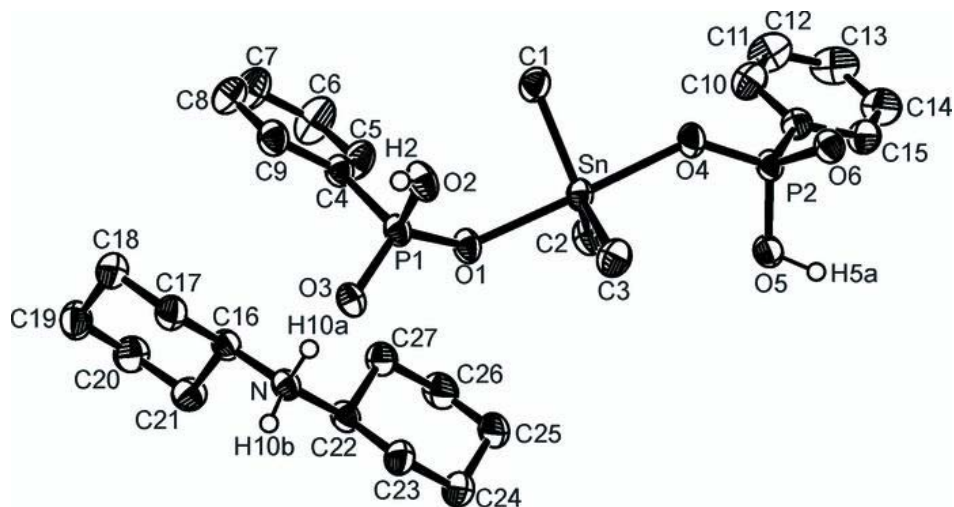


Fig. 2m

