

(2-Carbamoylethyl- κ^2C^1,O)triiodido-tin(IV)

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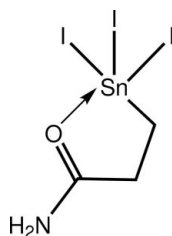
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Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(C-C) = 0.008$ Å; R factor = 0.027; wR factor = 0.079; data-to-parameter ratio = 27.1.

Two independent but virtually identical molecules comprise the asymmetric unit of the title compound, $[Sn(C_3H_6NO)I_3]$. The Cl_3O coordination geometry around the Sn^{IV} atom is defined by a chelating carbamoylethyl ligand (C^1,O -bidentate) and three I atoms, and is based on a distorted trigonal bipyramid with the carbonyl O atom occupying a position *trans* to one of the I atoms which forms the longer of the Sn–I bonds. The independent molecules are linked *via* N–H...O hydrogen bonds, which leads to the formation on an eight-membered amide $\{\cdots HNCO\}_2$ synthon. N–H...I hydrogen-bonding interactions are also present between neighbouring molecules.

Related literature

For background to and for related $Sn[OCH(NH_2)CH_2CH_2]Cl_3L$ structures ($L =$ amide), see: Howie *et al.* (2011*a,b*); Wardell *et al.* (2010); Tiekink *et al.* (2006). For additional geometric analysis, see: Addison *et al.* (1984); Spek (2009).



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Experimental

Crystal data

$[Sn(C_3H_6NO)I_3]$
 $M_r = 571.48$
 Triclinic, $P\bar{1}$
 $a = 7.8530$ (1) Å
 $b = 10.6264$ (1) Å
 $c = 14.1250$ (2) Å
 $\alpha = 98.801$ (1)°
 $\beta = 105.523$ (1)°
 $\gamma = 102.383$ (1)°
 $V = 1081.22$ (2) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 10.87$ mm⁻¹
 $T = 120$ K
 $0.20 \times 0.20 \times 0.02$ mm

Data collection

Bruker–Nonius APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2007)
 $T_{min} = 0.379$, $T_{max} = 1.000$
 14061 measured reflections
 4414 independent reflections
 4342 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.039$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$
 $wR(F^2) = 0.079$
 $S = 1.12$
 4414 reflections
 163 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 1.37$ e Å⁻³
 $\Delta\rho_{min} = -1.46$ e Å⁻³

Table 1

Selected bond lengths (Å).

Sn1–C1	2.146 (5)	Sn2–C4	2.147 (5)
Sn1–O1	2.347 (3)	Sn2–O2	2.330 (3)
Sn1–I1	2.6953 (4)	Sn2–I4	2.6987 (4)
Sn1–I2	2.7796 (4)	Sn2–I5	2.6880 (4)
Sn1–I3	2.6904 (4)	Sn2–I6	2.8060 (4)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1–H1n...O2	0.88	2.29	3.085 (7)	150
N2–H3n...O1	0.88	2.26	3.018 (7)	145
N2–H4n...I1	0.88	3.06	3.784 (6)	141

Data collection: COLLECT (Hooft, 1998); cell refinement: DENZO (Otwinowski & Minor, 1997) and COLLECT; data reduction: DENZO and COLLECT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997) and DIAMOND (Brandenburg, 2006); software used to prepare material for publication: pubCIF (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2541).

References

- Addison, A. W., Rao, T. N., Reedijk, J., van Rijn, J. & Verschoor, G. C. (1984). *J. Chem. Soc. Dalton Trans.* pp. 1349–1356.
- Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Hoof, R. W. W. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
- Howie, R. A., de Lima, G. M., Tiekink, E. R. T., Wardell, J. L. & Wardell, S. M. S. V. (2011*a*). *Acta Cryst.* **E67**, m1420–m1421.
- Howie, R. A., de Lima, G. M., Tiekink, E. R. T., Wardell, J. L., Wardell, S. M. S. V. & Welte, W. B. (2011*b*). *Z. Kristallogr.* doi:10.1524/zkri.2011.1440.
- Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
- Sheldrick, G. M. (2007). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
- Tiekink, E. R. T., Wardell, J. L. & Wardell, S. M. S. V. (2006). *Acta Cryst.* **E62**, m971–m973.
- Wardell, S. M. S. V., Harrison, W. T. A., Tiekink, E. R. T., de Lima, G. M. & Wardell, J. L. (2010). *Acta Cryst.* **E66**, m312–m313.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supplementary materials

Acta Cryst. (2011). E67, m1536-m1537 [doi:10.1107/S1600536811041778]

(2-Carbamoylethyl- κ^2C^1,O)triiodidotin(IV)

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Comment

The title compound, (I), was studied as a continuation of structural investigations of 2-amidoethyl compounds of stannanes(IV) (Tiekink *et al.*, 2006; Wardell *et al.*, 2010; Howie *et al.*, 2011*a,b*, and references therein).

Two independent molecules comprise the asymmetric unit of (I), (Fig. 1). The two molecules are virtually identical with the r.m.s. deviations for distances and angles being 0.0132 Å and 3.291°, respectively (Spek, 2009). The greatest difference in equivalent bond lengths is found in the Sn1—I2 and Sn2—I6 bonds (Table 1). The Sn^{IV} atom in each molecule is chelated by the amidoethyl ligand and additionally coordinated by three I atoms. Each of the five-membered chelate rings is twisted, with the twist occurring about the CH₂—CH₂ bond in each case. The resulting Cl₃O donor set defines a coordination geometry intermediate between square-pyramidal and trigonal-bipyramidal, with a leaning towards the latter description. This is quantified by the value of $\tau = 0.80$ [Sn1] which compares to the τ values of 0.0 and 1.0 for ideal square-pyramidal and trigonal-bipyramidal geometries, respectively (Addison *et al.*, 1984). The τ value for the Sn2 atom is 0.72. The disparity in the Sn—I bond lengths (Table 1), shows that the I atoms in the axial positions, each of which is *trans* to an O atom, form longer bonds than the I atoms occupying equatorial positions.

It is of interest that while (H₂NCOCH₂CH₂-C,O)SnCl₃ readily forms six-coordinate complexes, [(H₂NCOCH₂CH₂-C,O)SnCl₃.L] with oxygen ligands, L, *e.g.* L = amide, as illustrated by the isolation of [(H₂NCOCH₂CH₂-C,O)(EtCONH₂-O)SnCl₃] from reaction mixtures containing SnCl₂, HCl and H₂C=CHCONH₂ in Et₂O (Howie *et al.*, 2011*b*), the triiodido analogue is reluctant to form similar complexes. This is a consequence of the reduced Lewis acidity of the tin atom in iodidostannanes compared to chloridostannanes.

The two molecules comprising the asymmetric unit are linked *via* N—H...O hydrogen bonds, leading to the formation of an eight-membered {...HNCO}₂ synthon (Fig. 1, Table 2). The other H atom on each N forms an interaction with an I atom of the other molecule, in the the case of the N1—H2n atom, this distance is long at 3.14 Å.

Experimental

A solution of the complex, (H₂NCOCH₂CH₂—C,O)(EtCONH₂-O)SnCl₃ (0.74 g, 2 mmol), isolated from a reaction mixture containing SnCl₂, HCl and H₂C=CHCONH₂ in Et₂O (Howie *et al.*, 2011*b*), and sodium iodide (10 mmol) in acetone (30 ml) was refluxed for 3 h, filtered to remove sodium chloride and rotary evaporated. The residue was extracted into chloroform (30 ml), the organic solution was rotary evaporated and the resulting residue was recrystallized from ethanol to give the title compound, melting point 461–463 K. IR: $\nu(\text{C}=\text{O})$ 1660, 1581 cm⁻¹.

Refinement

The C-bound H atoms were geometrically placed (N—H = 0.88 Å and C—H = 0.99 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N}, \text{C})$. The maximum and minimum residual electron density peaks of 1.37 and 1.46 e⁻ Å⁻³, respectively, are located 1.34 Å and 0.85 Å from the I5 and I3 atoms, respectively.

Figures

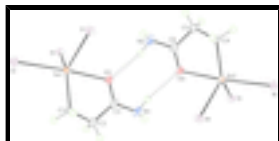


Fig. 1. The molecular structure of the two independent molecules comprising the asymmetric unit in (I) showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level. The N—H...O hydrogen bonds are shown as dashed lines.

(2-Carbamoylethyl-κ²C¹,O)triiodidotin(IV)

Crystal data

[Sn(C ₃ H ₆ NO) ₃]	$Z = 4$
$M_r = 571.48$	$F(000) = 992$
Triclinic, <i>PT</i>	$D_x = 3.511 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 7.8530 (1) \text{ \AA}$	Cell parameters from 4411 reflections
$b = 10.6264 (1) \text{ \AA}$	$\theta = 2.9\text{--}27.5^\circ$
$c = 14.1250 (2) \text{ \AA}$	$\mu = 10.87 \text{ mm}^{-1}$
$\alpha = 98.801 (1)^\circ$	$T = 120 \text{ K}$
$\beta = 105.523 (1)^\circ$	Plate, yellow
$\gamma = 102.383 (1)^\circ$	$0.20 \times 0.20 \times 0.02 \text{ mm}$
$V = 1081.22 (2) \text{ \AA}^3$	

Data collection

Bruker–Nonius APEXII CCD diffractometer	4414 independent reflections
Radiation source: Bruker–Nonius FR591 rotating anode	4342 reflections with $I > 2\sigma(I)$
10cm confocal mirrors	$R_{\text{int}} = 0.039$
Detector resolution: 9.091 pixels mm ⁻¹	$\theta_{\text{max}} = 26.5^\circ$, $\theta_{\text{min}} = 3.0^\circ$
φ and ω scans	$h = -9 \rightarrow 9$
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 2007)	$k = -13 \rightarrow 13$
$T_{\text{min}} = 0.379$, $T_{\text{max}} = 1.000$	$l = -17 \rightarrow 17$
14061 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.027$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.079$	H-atom parameters constrained
$S = 1.12$	$w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 3.8857P]$
4414 reflections	where $P = (F_o^2 + 2F_c^2)/3$
163 parameters	$(\Delta/\sigma)_{\max} = 0.001$
0 restraints	$\Delta\rho_{\max} = 1.37 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\min} = -1.46 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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	$U_{\text{iso}}^*/U_{\text{eq}}$
Sn1	0.84744 (4)	0.81052 (3)	0.07941 (2)	0.01343 (9)
I1	0.79233 (5)	0.56511 (3)	0.11465 (2)	0.02019 (10)
I2	1.13298 (5)	0.80096 (3)	-0.00043 (3)	0.02164 (10)
I3	0.58439 (4)	0.79311 (3)	-0.09302 (2)	0.01808 (9)
O1	0.6302 (5)	0.8274 (4)	0.1636 (3)	0.0196 (7)
N1	0.5852 (8)	0.9523 (5)	0.2928 (4)	0.0324 (12)
H1N	0.4849	0.8870	0.2762	0.039*
H2N	0.6529	0.9568	0.3546	0.039*
C1	0.9830 (7)	0.9848 (5)	0.1974 (4)	0.0190 (10)
H1A	1.0707	0.9634	0.2533	0.023*
H1B	1.0533	1.0528	0.1714	0.023*
C2	0.8454 (9)	1.0397 (5)	0.2370 (4)	0.0266 (12)
H2A	0.9052	1.0874	0.3083	0.032*
H2B	0.8057	1.1037	0.1978	0.032*
C3	0.6791 (7)	0.9313 (5)	0.2296 (4)	0.0198 (10)
Sn2	0.27996 (4)	0.67003 (3)	0.46025 (2)	0.01266 (9)
I4	0.61233 (4)	0.84602 (3)	0.54333 (3)	0.01904 (10)
I5	0.02318 (4)	0.80393 (3)	0.43118 (2)	0.01823 (9)

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I6	0.25104 (5)	0.60910 (3)	0.64270 (2)	0.02072 (10)
O2	0.3235 (5)	0.6994 (4)	0.3074 (3)	0.0208 (8)
N2	0.3498 (7)	0.5858 (5)	0.1668 (4)	0.0286 (11)
H3N	0.3856	0.6666	0.1585	0.034*
H4N	0.4401	0.5480	0.1716	0.034*
C4	0.2650 (7)	0.4737 (5)	0.3869 (4)	0.0171 (9)
H4A	0.3835	0.4533	0.4140	0.021*
H4B	0.1684	0.4090	0.4005	0.021*
C5	0.2215 (7)	0.4620 (5)	0.2734 (4)	0.0213 (11)
H5A	0.2708	0.3921	0.2449	0.026*
H5B	0.0868	0.4358	0.2414	0.026*
C6	0.3029 (7)	0.5905 (5)	0.2496 (4)	0.0188 (10)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01254 (17)	0.01471 (17)	0.01161 (16)	0.00316 (13)	0.00254 (13)	0.00162 (12)
I1	0.02194 (19)	0.01739 (17)	0.02113 (18)	0.00547 (14)	0.00490 (14)	0.00694 (13)
I2	0.01880 (18)	0.02449 (18)	0.02683 (19)	0.00877 (14)	0.01201 (14)	0.00795 (14)
I3	0.01449 (17)	0.02295 (18)	0.01437 (17)	0.00462 (13)	0.00081 (13)	0.00423 (13)
O1	0.0162 (18)	0.0241 (18)	0.0176 (17)	0.0048 (14)	0.0059 (14)	0.0023 (14)
N1	0.044 (3)	0.027 (2)	0.032 (3)	0.009 (2)	0.025 (2)	-0.001 (2)
C1	0.021 (3)	0.013 (2)	0.016 (2)	-0.0025 (19)	0.001 (2)	-0.0023 (18)
C2	0.045 (4)	0.016 (2)	0.024 (3)	0.010 (2)	0.018 (3)	0.003 (2)
C3	0.025 (3)	0.026 (3)	0.016 (2)	0.014 (2)	0.011 (2)	0.008 (2)
Sn2	0.01234 (17)	0.01365 (16)	0.01193 (16)	0.00425 (12)	0.00339 (13)	0.00231 (12)
I4	0.01251 (17)	0.01815 (17)	0.02403 (18)	0.00266 (13)	0.00420 (13)	0.00230 (13)
I5	0.01529 (18)	0.02042 (17)	0.02122 (18)	0.00887 (13)	0.00530 (13)	0.00606 (13)
I6	0.01956 (18)	0.02811 (19)	0.01277 (16)	0.00340 (14)	0.00347 (13)	0.00657 (13)
O2	0.028 (2)	0.0208 (18)	0.0155 (17)	0.0060 (15)	0.0108 (15)	0.0032 (14)
N2	0.035 (3)	0.030 (3)	0.022 (2)	0.005 (2)	0.015 (2)	0.003 (2)
C4	0.022 (3)	0.013 (2)	0.013 (2)	0.0072 (19)	0.0009 (19)	0.0001 (17)
C5	0.022 (3)	0.021 (2)	0.016 (2)	0.002 (2)	0.004 (2)	-0.0031 (19)
C6	0.014 (2)	0.029 (3)	0.016 (2)	0.009 (2)	0.0047 (19)	0.006 (2)

Geometric parameters (\AA , $^\circ$)

Sn1—C1	2.146 (5)	Sn2—C4	2.147 (5)
Sn1—O1	2.347 (3)	Sn2—O2	2.330 (3)
Sn1—I1	2.6953 (4)	Sn2—I4	2.6987 (4)
Sn1—I2	2.7796 (4)	Sn2—I5	2.6880 (4)
Sn1—I3	2.6904 (4)	Sn2—I6	2.8060 (4)
O1—C3	1.244 (6)	O2—C6	1.262 (6)
N1—C3	1.324 (7)	N2—C6	1.313 (6)
N1—H1N	0.8800	N2—H3N	0.8800
N1—H2N	0.8800	N2—H4N	0.8800
C1—C2	1.521 (7)	C4—C5	1.526 (7)
C1—H1A	0.9900	C4—H4A	0.9900
C1—H1B	0.9900	C4—H4B	0.9900

C2—C3	1.512 (8)	C5—C6	1.506 (7)
C2—H2A	0.9900	C5—H5A	0.9900
C2—H2B	0.9900	C5—H5B	0.9900
C1—Sn1—O1	76.52 (16)	C4—Sn2—O2	77.38 (16)
C1—Sn1—I3	125.92 (14)	C4—Sn2—I5	129.25 (14)
O1—Sn1—I3	87.71 (9)	O2—Sn2—I5	89.69 (9)
C1—Sn1—I1	122.64 (14)	C4—Sn2—I4	118.64 (14)
O1—Sn1—I1	83.18 (9)	O2—Sn2—I4	84.58 (9)
I3—Sn1—I1	105.788 (15)	I5—Sn2—I4	108.400 (14)
C1—Sn1—I2	98.50 (14)	C4—Sn2—I6	96.42 (13)
O1—Sn1—I2	173.92 (9)	O2—Sn2—I6	172.63 (9)
I3—Sn1—I2	98.106 (14)	I5—Sn2—I6	97.373 (13)
I1—Sn1—I2	96.853 (14)	I4—Sn2—I6	95.120 (13)
C3—O1—Sn1	112.5 (3)	C6—O2—Sn2	111.5 (3)
C3—N1—H1N	109.5	C6—N2—H3N	109.5
C3—N1—H2N	109.5	C6—N2—H4N	109.5
H1N—N1—H2N	109.5	H3N—N2—H4N	109.5
C2—C1—Sn1	111.0 (4)	C5—C4—Sn2	110.1 (3)
C2—C1—H1A	109.4	C5—C4—H4A	109.6
Sn1—C1—H1A	109.4	Sn2—C4—H4A	109.6
C2—C1—H1B	109.4	C5—C4—H4B	109.6
Sn1—C1—H1B	109.4	Sn2—C4—H4B	109.6
H1A—C1—H1B	108.0	H4A—C4—H4B	108.1
C3—C2—C1	111.7 (4)	C6—C5—C4	111.5 (4)
C3—C2—H2A	109.3	C6—C5—H5A	109.3
C1—C2—H2A	109.3	C4—C5—H5A	109.3
C3—C2—H2B	109.3	C6—C5—H5B	109.3
C1—C2—H2B	109.3	C4—C5—H5B	109.3
H2A—C2—H2B	107.9	H5A—C5—H5B	108.0
O1—C3—N1	121.5 (5)	O2—C6—N2	121.2 (5)
O1—C3—C2	120.3 (4)	O2—C6—C5	120.6 (4)
N1—C3—C2	118.2 (5)	N2—C6—C5	118.2 (5)
C1—Sn1—O1—C3	6.4 (4)	C4—Sn2—O2—C6	5.8 (3)
I3—Sn1—O1—C3	-121.4 (3)	I5—Sn2—O2—C6	-124.7 (3)
I1—Sn1—O1—C3	132.4 (3)	I4—Sn2—O2—C6	126.8 (3)
O1—Sn1—C1—C2	-19.9 (3)	O2—Sn2—C4—C5	-20.4 (3)
I3—Sn1—C1—C2	57.1 (4)	I5—Sn2—C4—C5	58.6 (4)
I1—Sn1—C1—C2	-92.5 (4)	I4—Sn2—C4—C5	-97.0 (3)
I2—Sn1—C1—C2	163.6 (3)	I6—Sn2—C4—C5	163.6 (3)
Sn1—C1—C2—C3	31.0 (6)	Sn2—C4—C5—C6	32.4 (5)
Sn1—O1—C3—N1	-172.4 (4)	Sn2—O2—C6—N2	-169.0 (4)
Sn1—O1—C3—C2	9.8 (6)	Sn2—O2—C6—C5	11.7 (6)
C1—C2—C3—O1	-27.7 (7)	C4—C5—C6—O2	-30.2 (7)
C1—C2—C3—N1	154.4 (5)	C4—C5—C6—N2	150.5 (5)

Hydrogen-bond geometry (Å, °)

D—H...A	D—H	H...A	D...A	D—H...A
N1—H1n...O2	0.88	2.29	3.085 (7)	150

supplementary materials

N2—H3n···O1	0.88	2.26	3.018 (7)	145
N2—H4n···I1	0.88	3.06	3.784 (6)	141

Fig. 1

