

# Di-*tert*-butyldiisothiocyanatotin(IV)

Anne Kamrowski and Hans Reuter\*

Chemistry, Osnabrück University, Barabarstr. 7, 49069 Osnabrück, Germany. \*Correspondence e-mail: hreuter@uos.de

Received 12 December 2024

Accepted 24 December 2024

Edited by W. T. A. Harrison, University of Aberdeen, United Kingdom

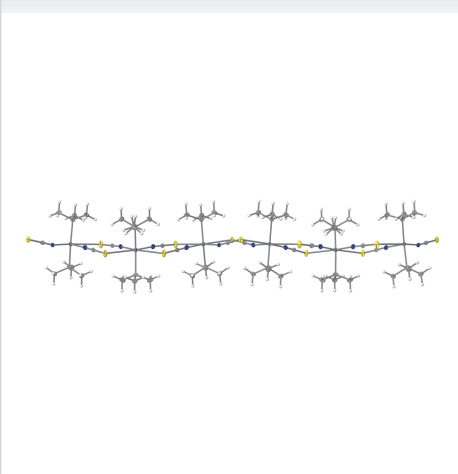
**Keywords:** crystal structure; isothiocyanate; intermolecular interactions; spherical coordinates; titling.

CCDC reference: 2412795

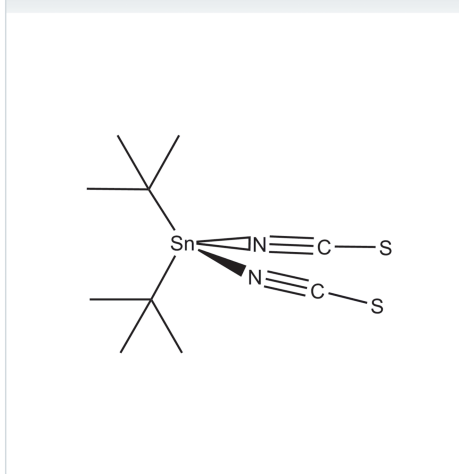
**Structural data:** full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

The title compound,  $[\text{Sn}(\text{C}_4\text{H}_9)_2(\text{NCS})_2]$ , which crystallizes with one and a half molecules in the asymmetric unit, represents a new structure type for intermolecular sulfur...tin interactions, which is characterized by an antiparallel (*A*) arrangement of the dipole moments of the individual molecules. In the resulting zigzag chains, the molecules are related to each other by mirror planes (*m*) and twofold rotation axes (*2*), both perpendicular to the propagation plane, while translation is realized *via* a glide plane in direction of the crystallographic *c* axis, a combination of symmetry elements unique in the structural chemistry of diorganotin(IV) dihalides and pseudohalides,  $R_2\text{SnX}_2$  with  $X = \text{Hal}$  or  $\text{NCS}$ . Its characteristics are subsumed in the term  $Am2c$  for this kind of intermolecular association pattern. The tilting of the  $\text{NSnN}$ -planes in relation to the propagation plane is described in terms of spherical coordinates.

## 3D view



## Chemical scheme



## Structure description

As linear, polyatomic pseudo-halide ion, the thiocyanate ion,  $\text{NCS}^-$ , is able to replace mono-atomic, spherical halide atoms in many compounds, which in the case of diorganotin(IV) dihalides,  $R_2\text{SnHal}_2$ , leads to the formation of the so-called diorganotin(IV) diisothiocyanates,  $R_2\text{Sn}(\text{NCS})_2$ , as the pseudo-halide ion binds to the 'hard' tin atom *via* its 'hard' nitrogen atom in accordance with the HSAB principle.

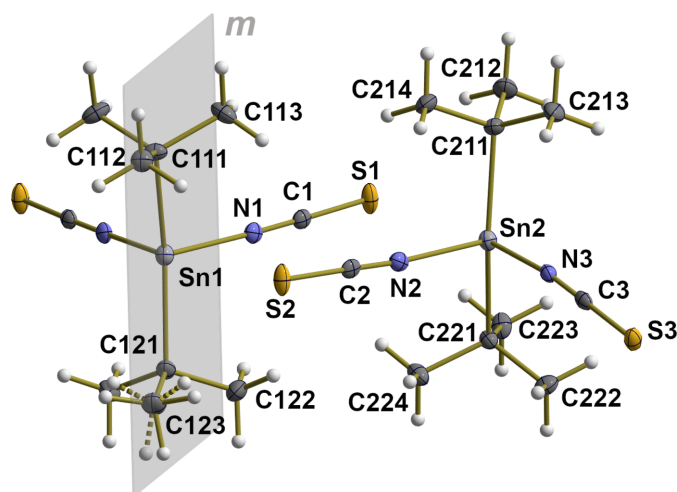
In terms of structural chemistry these compounds are of special interest with regard to their intermolecular interactions, which for steric reasons can only take place *via* the 'soft' sulfur atoms. In case of the methyl and ethyl compounds (Britton, 2006), these interactions result in a chain-like arrangement of the individual molecules with a parallel orientation of their dipole moments while the phenyl compound (Pancratz *et al.*, 2024) represents a di-periodic coordination polymer in which the molecules have lost their individuality. In search of a molecular *diisocyanate* we have prepared for the first time the title *tert*-butyl compound because the bulky *tert*-butyl substituents prevent an intermolecular association in the comparable *dichloride* (Dakternieks *et al.*, 1994).

## data reports

The title compound,  $\text{tBu}_2\text{Sn}(\text{NCS})_2$ , crystallizes in the orthorhombic space group  $Pbcm$  with 12 molecules in the unit cell and one and a half molecules in the asymmetric unit (Fig. 1). The half molecule results from a crystallographic mirror plane that bisects the tin atom and the two *tert*-butyl groups with order/disorder of the hydrogen atoms of the affected methyl group.

The carbon–carbon bond lengths within the *tert*-butyl groups [ $\text{C}–\text{C} = 1.514(7)–1.530(4) \text{ \AA}$ , mean value =  $1.525(6) \text{ \AA}$ ] are only slightly shorter than the value given in literature [ $d(\text{C}_{sp^3}–\text{CH}_3) = 1.534(11) \text{ \AA}$  (Allen *et al.*, 1987)]. The mean bond angles of  $110.1(4)^\circ$  between the methyl groups correspond very well with tetrahedrally coordinated,  $sp^3$ -hybridized carbon atoms. With the tin–carbon–carbon bond angles, it is noticeable that in each *tert*-butyl group two angles are smaller [mean value:  $107.1(4)^\circ$ ] than the third one [mean value:  $110.1(9)^\circ$ ].

The bond lengths and angles describing the coordination sphere of the tin atoms, however, have very unusual values. Thus, the Sn–C distances of  $2.214(4)–2.227(3) \text{ \AA}$  [mean value:  $2.221(6) \text{ \AA}$ ] are quite long and the bond angles of  $157.3(2)/157.2(2)^\circ$  between the *tert*-butyl groups are greatly widened in comparison with the corresponding values [ $2.149(4)/2.151(4) \text{ \AA}$ ,  $133.1(2)^\circ$ ] in the crystal structure of the parent compound di-*tert*-butyltin(IV) dichloride,  $\text{tBu}_2\text{SnCl}_2$  (Dakternieks *et al.*, 1994). The same applies to the bond angles between the inorganic ligands which are considerably smaller in the title compound [ $84.4(1)^\circ/84.7(1)^\circ$ ] than in the dichloride [ $101.86(5)^\circ$ ], an effect that can be attributed to the smaller size of the nitrogen atoms in comparison with the chloride ions. Similar changes of bond angles are found in compounds  $\text{R}_2\text{SnX}_2$  with  $\text{R} = \text{Me}$  and  $\text{Et}$ , respectively when



**Figure 1**

Ball-and-stick model of the tetrahedral environment of the two crystallographically independent  $\text{tBu}_2\text{Sn}(\text{NCS})_2$  molecules with atom numbering given for the asymmetric unit and orientation of the crystallographic mirror plane,  $m$ , in the molecule of Sn1. With the exception of the hydrogen atoms, which are shown as spheres of arbitrary radius, all other atoms are drawn as displacement ellipsoids at the 40% probability level. Disorder of the hydrogen atoms attached to C123 is shown by dashed bonds in the case of the second hydrogen-atom orientation.

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Sn1–N1	2.180 (3)	Sn1–C111	2.224 (4)
Sn2–N2	2.172 (3)	S1–Sn2	3.1519 (9)
Sn2–N3	2.175 (3)	S2–Sn1	3.1312 (9)
Sn1–C121	2.214 (4)	S3–Sn2 <sup>i</sup>	3.1355 (9)
C1–N1–Sn1	174.6 (2)	C3–N3–Sn2	167.0 (2)
C2–N2–Sn2	175.2 (3)		

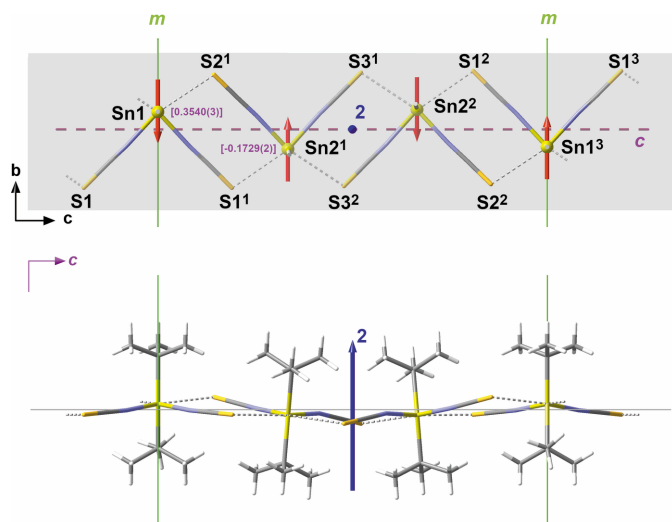
Symmetry code: (i)  $x, -y + \frac{1}{2}, -z$ .

comparing  $X = \text{Cl}$  and  $X = \text{NCS}$ . For  $\text{R} = \text{Me}$ ,  $\langle(\text{C}–\text{Sn}–\text{C})$  changes from  $142.2(4)^\circ$  for  $X = \text{Cl}$  (Reuter & Pawlak, 2001) to  $147.6(1)^\circ$  (Britton, 2006) and  $\langle(X–\text{Sn}–X)$  from  $98.60(9)^\circ$  to  $86.08(8)^\circ$  for  $X = \text{NCS}$  (Britton, 2006)], and for  $\text{R} = \text{Et}$ ,  $\langle(\text{C}–\text{Sn}–\text{C})$  changes from  $134.0(6)^\circ$  for  $X = \text{Cl}$  (Alcock & Sawyer, 1977) to  $153.03(6)^\circ$  for  $X = \text{NCS}$  (Britton, 2006) and  $\langle(X–\text{Sn}–X)$  from  $96.0(1)^\circ$  to  $83.57(8)^\circ$  for  $X = \text{NCS}$ . The tin–carbon bond lengths, however, differ only slightly in the compounds in question.

The bond lengths [mean  $\text{N}–\text{C} = 1.103(3) \text{ \AA}$ , mean  $\text{C}–\text{S} = 1.627(4) \text{ \AA}$ ] and angles [mean  $\langle(\text{N}–\text{C}–\text{S}) = 178.5(3)^\circ$ ] within the almost linear isothiocyanate groups are only slightly affected by their coordination behavior (Table 1) and almost identical with the values found in the other structurally determined *diisothiocyanates* [ $\text{R} = \text{Me}$ ,  $\text{Et}$  (Britton, 2006),  $\text{R} = \text{Ph}$  (Pancratz *et al.*, 2024)]. These values correspond very well with a formal carbon–nitrogen triple [ $d(\text{C}_{sp}–\text{N}) = 1.155(12) \text{ \AA}$  (Allen *et al.*, 1987)] and a carbon–sulfur single [ $d(\text{C}_{sp}–\text{S}) = 1.630(14) \text{ \AA}$  (Allen *et al.*, 1987)] bond. Their coordination to the tin atoms *via* the nitrogen atoms is characterized by a mean tin–nitrogen distance of  $2.176(5) \text{ \AA}$  over all four NCS groups but the Sn–N–C bond angles show a greater variance. Three of the four bond angles are around  $174.5(8)^\circ$  while one only reaches  $167.0(2)^\circ$  (Table 1).

Despite the widening of the bond angles between the *tert*-butyl groups, intermolecular tin–sulfur distances [ $3.1312(9)–3.1519(9) \text{ \AA}$ ] are of the same order of magnitude as in the corresponding methyl [ $3.146(1) \text{ \AA}$ ] and ethyl [ $3.060(1) \text{ \AA}$ ] compounds (Britton, 2006) and thus significantly longer than in  $\text{Ph}_2\text{Sn}(\text{NCS})_2$  [ $2.7224(5) \text{ \AA}$ ; Pancratz *et al.*, 2024]. In relation to the sum ( $2.43 \text{ \AA}$ ) of the covalent radii (Cordero *et al.*, 2008) of tin ( $1.39 \text{ \AA}$ ) and sulfur ( $1.04 \text{ \AA}$ ), these secondary tin–sulfur contact lengths of around  $3.1 \text{ \AA}$  are quite long ( $+0.67 \text{ \AA} = +28\%$ ) but in relation to the sum ( $3.97 \text{ \AA}$ ) of the van der Waals radii (Mantina *et al.*, 2009) of tin ( $2.17 \text{ \AA}$ ) and sulfur ( $1.80 \text{ \AA}$ ) quite short ( $-0.87 \text{ \AA} = 22\%$ ). In summary, these secondary contacts lead to a chain-like arrangement of the individual molecules with anti-parallel arrangement of the dipole moments and carbon–sulfur···tin angles of  $99.8(1)–100.7(1)^\circ$  (Fig. 2).

Within the zigzag-chains the two molecules are related to each other by a sequence of mirror planes,  $m$ , and twofold rotation axes,  $2$ , all perpendicular to the propagation plane parallel to the crystallographic  $a$  and  $b$  axes, while translation of the molecules is arranged *via* the glide plane  $c$  from which the tin atoms are at different distances (Fig. 2). The repeat unit therefore corresponds to the length of the  $c$  axis =



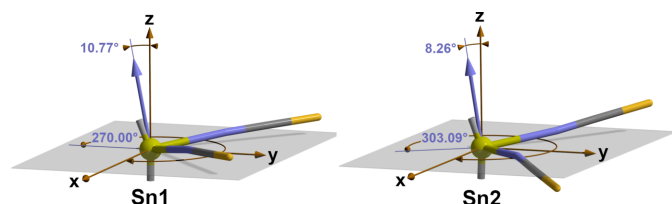
**Figure 2**

Schematic, ball-and-stick representation of the antiparallel, chain-like arrangement of the dipole moments (red arrows of arbitrary units, orientation assumed in the direction of the center point between the two nitrogen atoms) of the  ${}^t\text{Bu}_2\text{Sn}(\text{NCS})_2$  molecules as a result of the tin···sulfur interactions (dashed sticks in gray) and their relation to the crystallographic symmetry elements: mirror plane =  $m$ , green line; twofold rotation axis perpendicular to the gray propagation plane =  $2$ , blue arrow; axial glide plane =  $c$ , dashed line, violet; above = top view on the propagation plane with organic groups omitted for clarity, below = side view; values in square brackets = distances (Å) of the tin atoms from the glide plane; atom color code used: Sn = bronze, N = blue, C = black, S = yellow, H = white; symmetry transformations used to generate equivalent atoms: (1)  $x, y, \frac{1}{2} - z$ ; (2)  $x, \frac{1}{2} - y, \frac{1}{2} + z$ ; (3)  $x, \frac{1}{2} - y, 1 - z$ .

36.0164 (9) Å. According to the classification scheme developed earlier (Ye & Reuter, 2012) based on the parallel ( $P$ ) or anti-parallel ( $A$ ) arrangement of the dipole moments and the symmetry elements involved in the intermolecular association, the present structure type can be denoted as  $Am2c$ .

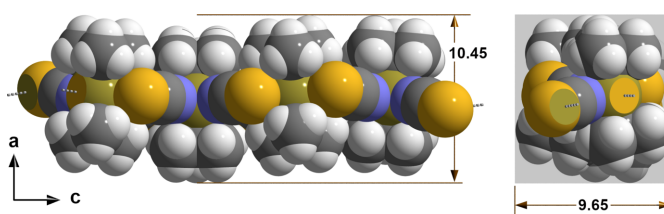
In the structural chemistry of diorganotin dihalides,  $R_2\text{SnHal}_2$ , anti-parallel arrangements of the dipole moments into zigzag chains are relatively common, but do not occur in the present combination ( $2, m$ ) of symmetry elements:  $\text{Me}_2\text{SnCl}_2 = Amm2_1$  (Reuter & Pawlak, 2001),  $\text{Et}_2\text{SnBr}_2 = A22_1$  (Alcock & Sawyer, 1977),  ${}^t\text{Bu}_2\text{SnCl}_2 = A2_1$  (Sawyer, 1988),  $\text{Et}_2\text{SnCl}_2 = Ac$  (Alcock & Sawyer, 1977).

As can easily be seen in Figs. 1 and 2, the N–Sn–N planes of the two molecules are not coplanar to the propagation plane. Quantitatively, the out-of-plane orientation of these



**Figure 3**

Spherical coordinate system used to calculate the spherical coordinates  $\Theta$  and  $\varphi$  in order to characterize the tilting of the NSnN-planes of both molecules in relation to the propagation plane (gray), arbitrary values for the authoritative normal vector  $N_{\text{NSnN}}$  (blue); for clarity the positions of the organic ligands are only indicated by short sticks.



**Figure 4**

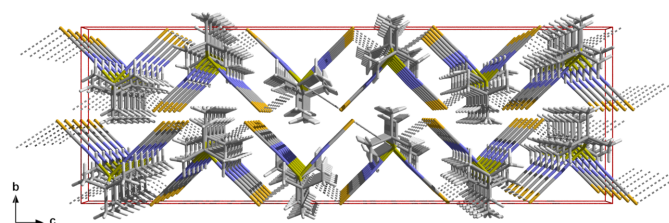
Detail of the chain-like arrangement of the  ${}^t\text{Bu}_2\text{Sn}(\text{NCS})_2$  molecules as space-filling model with dimensions in Å; left side = side view looking down the  $b$  axis, right side = front view; atoms are represented as single-colored or truncated, two-colored spheres according to their van der Waals radii and cut-offs based on the intersection of the two spheres with cut-off faces showing the color of the interpenetrating atom, intermolecular tin···sulfur contacts are visualized as dashed sticks in gray; atom color code used: Sn = bronze, N = blue, C = black, S = yellow, H = white.

planes can be described in terms of spherical coordination systems defined by the radial distance  $r$ , the polar angle  $\Theta$  and the azimuthal angle  $\varphi$  (Fig. 3): with the tin atom as origin,  $r$  as the lengths of the normal vector  $N_{\text{NSnN}}$ ,  $\Theta$  as the angle between this normal vector and the polar axis  $z$  (= the crystallographic  $a$  axis) and  $\varphi$  as the angle of rotation around the polar axis  $z$  in the meridional  $xy$  plane (= plane through Sn and coplanar to the propagation plane  $bc$ ). The corresponding values are  $\Theta = 10.77^\circ$ ,  $\varphi = 270^\circ$  for the NSnN plane of Sn1, and  $\Theta = 8.26^\circ$ ,  $\varphi = 303.09^\circ$  for the NSnN plane of Sn2.

Including the organic residuals into account the sinusoidal chains have an almost rectangular cross-section (Fig. 4) of about  $9.65 \times 10.45$  Å and are arranged in the direction of the  $b$  axis whereby the wave crest of the one chain engaged in the wave valley of the other one (Fig. 5). For an interpretation of the secondary contacts in terms of  $3c-4e$  bonds see Alcock & Sawyer (1977).

### Synthesis and crystallization

The synthesis was carried out according to a published protocol from sodium thiocyanate and di-*tert*-butyltin(IV) dichloride,  ${}^t\text{Bu}_2\text{SnCl}_2$ , (Kandil & Allred, 1970) in ethanol (molar ratio 1:2): colorless, needle-like single crystals were obtained after recrystallization from toluene solution.



**Figure 5**

Ball-and-stick representation showing the molecule packing and interlocking of the chains formed when looking down the  $a$  axis; intermolecular tin···sulfur contacts are shown as dashed sticks in gray.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

## Acknowledgements

We thank the Deutsche Forschungsgemeinschaft and the Government of Lower-Saxony for funding the diffractometer and acknowledge support by the Deutsche Forschungsgemeinschaft (DFG).

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**Table 2**

Experimental details.

Crystal data	
Chemical formula	[Sn(C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> (NCS) <sub>2</sub> ]
<i>M<sub>r</sub></i>	349.07
Crystal system, space group	Orthorhombic, <i>Pbcm</i>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.6669 (3), 11.9440 (4), 36.0164 (9)
<i>V</i> (Å <sup>3</sup> )	4158.5 (2)
<i>Z</i>	12
Radiation type	Mo <i>K</i> α
$\mu$ (mm <sup>-1</sup> )	2.12
Crystal size (mm)	0.18 × 0.12 × 0.06
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan ( <i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>	0.697, 0.891
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	169441, 5093, 4052
<i>R</i> <sub>int</sub>	0.104
(sin θ/λ) <sub>max</sub> (Å <sup>-1</sup> )	0.661
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.033, 0.067, 1.12
No. of reflections	5093
No. of parameters	225
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ (e Å <sup>-3</sup> )	0.62, -1.01

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS97* (Sheldrick 2008), *SHELXL2014/7* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2006), *Mercury* (Macrae *et al.* (2020)), *POVRAY* (Povray, 2004) and *pubCIF* (Westrip, 2010).

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## full crystallographic data

*IUCrData* (2025). **10**, x241244 [<https://doi.org/10.1107/S2414314624012446>]

Di-*tert*-butyldiisothiocyanatotin(IV)

Anne Kamrowski and Hans Reuter

Di-*tert*-butyldiisothiocyanatotin(IV)*Crystal data*

[Sn(C<sub>4</sub>H<sub>9</sub>)<sub>2</sub>(NCS)<sub>2</sub>]

*M<sub>r</sub>* = 349.07

Orthorhombic, *Pbcm*

*a* = 9.6669 (3) Å

*b* = 11.9440 (4) Å

*c* = 36.0164 (9) Å

*V* = 4158.5 (2) Å<sup>3</sup>

*Z* = 12

*F*(000) = 2088

*D<sub>x</sub>* = 1.673 Mg m<sup>-3</sup>

Mo *Kα* radiation, *λ* = 0.71073 Å

Cell parameters from 9996 reflections

*θ* = 2.4–29.2°

*μ* = 2.12 mm<sup>-1</sup>

*T* = 100 K

Plate, colourless

0.18 × 0.12 × 0.06 mm

*Data collection*

Bruker APEXII CCD

diffractometer

*φ* and *ω* scans

Absorption correction: multi-scan

(SADABS; Krause *et al.*, 2015)

*T<sub>min</sub>* = 0.697, *T<sub>max</sub>* = 0.891

169441 measured reflections

5093 independent reflections

4052 reflections with *I* > 2σ(*I*)

*R<sub>int</sub>* = 0.104

*θ<sub>max</sub>* = 28.0°, *θ<sub>min</sub>* = 2.1°

*h* = -12→12

*k* = -15→15

*l* = -47→47

*Refinement*

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

Least-squares matrix: full

*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.033

*wR*(*F*<sup>2</sup>) = 0.067

*S* = 1.12

5093 reflections

225 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Hydrogen site location: mixed

H-atom parameters constrained

*w* = 1/[σ<sup>2</sup>(*F<sub>o</sub>*<sup>2</sup>) + (0.0162*P*)<sup>2</sup> + 7.7574*P*]

where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3

(Δ/σ)<sub>max</sub> = 0.001

Δρ<sub>max</sub> = 0.62 e Å<sup>-3</sup>

Δρ<sub>min</sub> = -1.01 e Å<sup>-3</sup>

Extinction correction: *SHELXL2014/7*

(Sheldrick 2015),

*F<sub>c</sub>*\* = *kF<sub>c</sub>*[1 + 0.001*xF<sub>c</sub>*<sup>2</sup>*λ*<sup>3</sup>/sin(2*θ*)]<sup>-1/4</sup>

Extinction coefficient: 0.00019 (2)

*Special details*

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

**Refinement.** The H atoms were geometrically placed (C—H = 0.98 Å) and refined as riding atoms. The *U*<sub>iso</sub> values for the H atoms were constrained to be the same for all atoms attached to a particular carbon atom.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Sn1	0.71338 (3)	0.31769 (2)	0.2500	0.01406 (8)	
C111	0.4833 (4)	0.3193 (4)	0.2500	0.0186 (9)	
C112	0.4302 (5)	0.4399 (4)	0.2500	0.0220 (10)	
H111	0.3289	0.4393	0.2500	0.030 (5)*	
H112	0.4636	0.4782	0.2277	0.030 (5)*	
C113	0.4340 (3)	0.2588 (3)	0.21517 (10)	0.0264 (8)	
H114	0.4663	0.1810	0.2157	0.030 (5)*	
H115	0.4713	0.2964	0.1932	0.030 (5)*	
H116	0.3327	0.2600	0.2142	0.030 (5)*	
C121	0.9254 (5)	0.3877 (4)	0.2500	0.0204 (10)	
C122	0.9991 (3)	0.3436 (3)	0.21538 (10)	0.0272 (8)	
H124	1.0943	0.3718	0.2149	0.039 (6)*	
H125	0.9500	0.3692	0.1931	0.039 (6)*	
H126	1.0002	0.2616	0.2159	0.039 (6)*	
C123	0.9251 (5)	0.5145 (4)	0.2500	0.0302 (11)	
H121	0.8625	0.5417	0.2694	0.039 (6)*	0.5
H122	0.8936	0.5418	0.2258	0.039 (6)*	0.5
H123	1.0189	0.5420	0.2548	0.039 (6)*	0.5
N1	0.7446 (3)	0.1848 (2)	0.20936 (8)	0.0187 (6)	
C1	0.7531 (3)	0.1200 (3)	0.18662 (9)	0.0173 (6)	
S1	0.76537 (10)	0.02369 (7)	0.15494 (2)	0.0272 (2)	
Sn2	0.76789 (2)	0.17360 (2)	0.08292 (2)	0.01418 (7)	
C211	0.5510 (3)	0.1151 (3)	0.07802 (9)	0.0199 (7)	
C212	0.5441 (4)	-0.0125 (3)	0.07864 (10)	0.0311 (8)	
H211	0.5816	-0.0401	0.1022	0.037 (4)*	
H212	0.5986	-0.0427	0.0580	0.037 (4)*	
H213	0.4476	-0.0365	0.0761	0.037 (4)*	
C213	0.4912 (3)	0.1599 (3)	0.04175 (10)	0.0269 (8)	
H214	0.3949	0.1352	0.0392	0.037 (4)*	
H215	0.5455	0.1314	0.0208	0.037 (4)*	
H216	0.4945	0.2419	0.0419	0.037 (4)*	
C214	0.4711 (3)	0.1641 (3)	0.11074 (10)	0.0259 (8)	
H217	0.4750	0.2460	0.1097	0.037 (4)*	
H218	0.5124	0.1381	0.1340	0.037 (4)*	
H219	0.3744	0.1396	0.1095	0.037 (4)*	
C221	0.9969 (3)	0.1591 (3)	0.08795 (9)	0.0179 (6)	
C222	1.0614 (3)	0.2197 (3)	0.05478 (10)	0.0244 (7)	
H221	1.1624	0.2168	0.0567	0.030 (3)*	
H222	1.0310	0.2980	0.0546	0.030 (3)*	
H223	1.0321	0.1832	0.0317	0.030 (3)*	
C223	1.0396 (3)	0.0371 (3)	0.08825 (9)	0.0242 (7)	
H224	1.0102	0.0014	0.0651	0.030 (3)*	
H225	0.9959	-0.0009	0.1093	0.030 (3)*	
H226	1.1404	0.0319	0.0906	0.030 (3)*	
C224	1.0400 (3)	0.2158 (3)	0.12421 (10)	0.0253 (8)	

H227	0.9974	0.1767	0.1452	0.030 (3)*
H228	1.0092	0.2940	0.1240	0.030 (3)*
H229	1.1409	0.2132	0.1266	0.030 (3)*
N2	0.7361 (3)	0.3049 (2)	0.12375 (8)	0.0188 (6)
C2	0.7134 (3)	0.3682 (3)	0.14610 (9)	0.0162 (6)
S2	0.68141 (10)	0.46205 (7)	0.17794 (2)	0.0266 (2)
N3	0.7594 (2)	0.3092 (2)	0.04267 (7)	0.0165 (5)
C3	0.7802 (3)	0.3744 (3)	0.02045 (9)	0.0169 (6)
S3	0.80855 (9)	0.46981 (7)	-0.01082 (2)	0.02275 (18)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Sn1	0.01571 (14)	0.01359 (16)	0.01288 (16)	0.00193 (11)	0.000	0.000
C111	0.0151 (19)	0.014 (2)	0.026 (3)	0.0000 (17)	0.000	0.000
C112	0.022 (2)	0.019 (2)	0.025 (3)	0.0045 (18)	0.000	0.000
C113	0.0204 (15)	0.0235 (18)	0.035 (2)	0.0015 (13)	-0.0095 (14)	-0.0094 (16)
C121	0.025 (2)	0.019 (2)	0.018 (2)	-0.0062 (18)	0.000	0.000
C122	0.0235 (15)	0.035 (2)	0.0227 (18)	-0.0030 (14)	0.0054 (14)	0.0016 (16)
C123	0.035 (3)	0.025 (3)	0.030 (3)	-0.010 (2)	0.000	0.000
N1	0.0214 (12)	0.0194 (15)	0.0152 (14)	0.0004 (11)	-0.0017 (10)	0.0047 (11)
C1	0.0181 (14)	0.0176 (16)	0.0162 (16)	0.0007 (12)	-0.0007 (12)	0.0057 (14)
S1	0.0499 (5)	0.0171 (4)	0.0147 (4)	0.0030 (4)	0.0006 (4)	-0.0018 (3)
Sn2	0.01568 (10)	0.01317 (11)	0.01369 (12)	0.00127 (8)	-0.00043 (7)	-0.00038 (8)
C211	0.0165 (14)	0.0216 (17)	0.0216 (17)	-0.0045 (12)	0.0005 (12)	0.0006 (14)
C212	0.0357 (19)	0.027 (2)	0.030 (2)	-0.0129 (16)	0.0020 (16)	-0.0025 (16)
C213	0.0198 (15)	0.039 (2)	0.0220 (18)	-0.0028 (14)	-0.0047 (13)	0.0009 (16)
C214	0.0218 (15)	0.032 (2)	0.0239 (19)	-0.0044 (14)	0.0062 (13)	0.0030 (15)
C221	0.0159 (13)	0.0193 (16)	0.0184 (17)	0.0027 (12)	-0.0013 (12)	-0.0033 (13)
C222	0.0194 (15)	0.0260 (19)	0.028 (2)	0.0009 (13)	0.0052 (14)	0.0009 (15)
C223	0.0262 (17)	0.0254 (19)	0.0211 (18)	0.0105 (14)	-0.0016 (13)	-0.0025 (14)
C224	0.0207 (16)	0.0287 (19)	0.0264 (19)	0.0039 (13)	-0.0053 (13)	-0.0094 (15)
N2	0.0205 (12)	0.0184 (14)	0.0176 (15)	-0.0020 (10)	-0.0025 (11)	0.0044 (12)
C2	0.0175 (14)	0.0151 (15)	0.0159 (17)	0.0008 (12)	-0.0010 (12)	0.0079 (13)
S2	0.0458 (5)	0.0190 (4)	0.0149 (4)	0.0104 (4)	0.0003 (4)	-0.0016 (3)
N3	0.0167 (12)	0.0187 (14)	0.0140 (14)	0.0002 (10)	-0.0017 (10)	-0.0032 (11)
C3	0.0159 (13)	0.0163 (16)	0.0185 (17)	0.0025 (12)	-0.0020 (12)	-0.0079 (13)
S3	0.0336 (4)	0.0198 (4)	0.0149 (4)	-0.0062 (3)	0.0004 (3)	0.0011 (3)

*Geometric parameters (Å, °)*

Sn1—N1 <sup>i</sup>	2.180 (3)	Sn2—C221	2.227 (3)
Sn1—N1	2.180 (3)	C211—C212	1.525 (5)
Sn2—N2	2.172 (3)	C211—C213	1.526 (5)
Sn2—N3	2.175 (3)	C211—C214	1.526 (4)
Sn1—C121	2.214 (4)	C212—H211	0.9800
Sn1—C111	2.224 (4)	C212—H212	0.9800
S1—Sn2	3.1519 (9)	C212—H213	0.9800



S2—Sn1	3.1312 (9)	C213—H214	0.9800
S3—Sn2 <sup>ii</sup>	3.1355 (9)	C213—H215	0.9800
C111—C113	1.524 (4)	C213—H216	0.9800
C111—C113 <sup>i</sup>	1.524 (4)	C214—H217	0.9800
C111—C112	1.529 (6)	C214—H218	0.9800
C112—H111	0.9800	C214—H219	0.9800
C112—H112	0.9799	C221—C223	1.514 (4)
C113—H114	0.9800	C221—C224	1.529 (4)
C113—H115	0.9800	C221—C222	1.530 (4)
C113—H116	0.9800	C222—H221	0.9800
C121—C123	1.514 (7)	C222—H222	0.9800
C121—C122 <sup>i</sup>	1.529 (4)	C222—H223	0.9800
C121—C122	1.530 (4)	C223—H224	0.9800
C122—H124	0.9800	C223—H225	0.9800
C122—H125	0.9800	C223—H226	0.9800
C122—H126	0.9800	C224—H227	0.9800
C123—H121	0.9800	C224—H228	0.9800
C123—H122	0.9800	C224—H229	0.9800
C123—H123	0.9800	N2—C2	1.126 (4)
N1—C1	1.130 (4)	C2—S2	1.633 (3)
C1—S1	1.625 (3)	N3—C3	1.134 (4)
Sn2—C211	2.217 (3)	C3—S3	1.625 (3)
N1 <sup>i</sup> —Sn1—N1	84.35 (13)	C211—Sn2—S1	83.05 (9)
N1 <sup>i</sup> —Sn1—C121	98.45 (11)	C221—Sn2—S1	84.07 (8)
N1—Sn1—C121	98.45 (11)	C212—C211—C213	110.3 (3)
N1 <sup>i</sup> —Sn1—C111	98.31 (10)	C212—C211—C214	110.5 (3)
N1—Sn1—C111	98.31 (10)	C213—C211—C214	109.5 (3)
C121—Sn1—C111	157.3 (2)	C212—C211—Sn2	110.8 (2)
N1 <sup>i</sup> —Sn1—S2	166.19 (7)	C213—C211—Sn2	108.4 (2)
N1—Sn1—S2	81.84 (7)	C214—C211—Sn2	107.2 (2)
C121—Sn1—S2	83.30 (7)	C211—C212—H211	109.5
C111—Sn1—S2	84.06 (6)	C211—C212—H212	109.5
C113—C111—C113 <sup>i</sup>	110.8 (4)	H211—C212—H212	109.5
C113—C111—C112	110.0 (2)	C211—C212—H213	109.5
C113 <sup>i</sup> —C111—C112	110.0 (2)	H211—C212—H213	109.5
C113—C111—Sn1	108.0 (2)	H212—C212—H213	109.5
C113 <sup>i</sup> —C111—Sn1	108.0 (2)	C211—C213—H214	109.5
C112—C111—Sn1	110.1 (3)	C211—C213—H215	109.5
C111—C112—H111	109.2	H214—C213—H215	109.5
C111—C112—H112	109.2	C211—C213—H216	109.5
H111—C112—H112	109.4	H214—C213—H216	109.5
C111—C113—H114	109.5	H215—C213—H216	109.5
C111—C113—H115	109.5	C211—C214—H217	109.5
H114—C113—H115	109.5	C211—C214—H218	109.5
C111—C113—H116	109.5	H217—C214—H218	109.5
H114—C113—H116	109.5	C211—C214—H219	109.5
H115—C113—H116	109.5	H217—C214—H219	109.5



C123—C121—C122 <sup>i</sup>	110.2 (3)	H218—C214—H219	109.5
C123—C121—C122	110.2 (3)	C223—C221—C224	110.2 (3)
C122 <sup>i</sup> —C121—C122	109.2 (4)	C223—C221—C222	110.5 (3)
C123—C121—Sn1	112.1 (3)	C224—C221—C222	110.2 (3)
C122 <sup>i</sup> —C121—Sn1	107.5 (2)	C223—C221—Sn2	110.3 (2)
C122—C121—Sn1	107.5 (2)	C224—C221—Sn2	107.8 (2)
C121—C122—H124	109.5	C222—C221—Sn2	107.8 (2)
C121—C122—H125	109.5	C221—C222—H221	109.5
H124—C122—H125	109.5	C221—C222—H222	109.5
C121—C122—H126	109.5	H221—C222—H222	109.5
H124—C122—H126	109.5	C221—C222—H223	109.5
H125—C122—H126	109.5	H221—C222—H223	109.5
C121—C123—H121	109.5	H222—C222—H223	109.5
C121—C123—H122	109.5	C221—C223—H224	109.5
H121—C123—H122	109.5	C221—C223—H225	109.5
C121—C123—H123	109.5	H224—C223—H225	109.5
H121—C123—H123	109.5	C221—C223—H226	109.5
H122—C123—H123	109.5	H224—C223—H226	109.5
C1—N1—Sn1	174.6 (2)	H225—C223—H226	109.5
C1—S1—Sn2	100.2 (1)	C221—C224—H227	109.5
C2—N2—Sn2	175.2 (3)	C221—C224—H228	109.5
C3—N3—Sn2	167.0 (2)	H227—C224—H228	109.5
N2—Sn2—N3	84.73 (10)	C221—C224—H229	109.5
N2—Sn2—C211	98.51 (11)	H227—C224—H229	109.5
N3—Sn2—C211	98.41 (10)	H228—C224—H229	109.5
N2—Sn2—C221	98.13 (10)	N1—C1—S1	178.2 (3)
N3—Sn2—C221	98.59 (10)	N2—C2—S2	178.8 (3)
C211—Sn2—C221	157.2 (1)	C2—S2—Sn1	100.7 (1)
N2—Sn2—S1	81.48 (7)	N3—C3—S3	178.8 (3)
N3—Sn2—S1	166.20 (7)	C3—S3—Sn2 <sup>ii</sup>	99.8 (1)

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