Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[trimethyltin(IV)]-μ-1,2,3-benzotriazol-1-ido-$\kappa^2N^1:N^3$]

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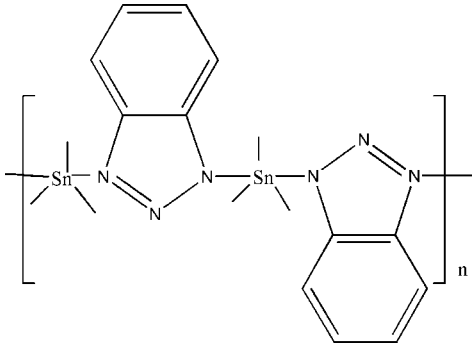
Received 20 December 2011; accepted 22 December 2011

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.016 Å; R factor = 0.030; wR factor = 0.137; data-to-parameter ratio = 15.7.

In the title coordination polymer, $[Sn(CH_3)_3(C_6H_4N_3)]_n$, the Sn^{IV} atom is five-coordinated in a distorted trigonal–bipyramidal geometry with the methyl groups in equatorial positions and two N atoms of two symmetry-related benzotriazolide anions in axial positions. The anion bridges adjacent metal atoms, forming zigzag polymeric chains parallel to [011] and [0$\bar{1}$1].

Related literature

For the biological activity of organotin complexes with nitrogen donor ligands, see: Pettinari *et al.* (1996). For related structures, see: Blaschette *et al.* (1992); Wirth *et al.* (1998); Berceanc *et al.* (2002).



Experimental

Crystal data

$[Sn(CH_3)_3(C_6H_4N_3)]$
M_r = 281.93
Orthorhombic, $Pna2_1$
a = 14.8168 (14) Å
b = 10.6687 (9) Å
c = 7.3518 (7) Å
V = 1162.14 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.16 mm^{-1}
T = 298 K
0.48 × 0.41 × 0.35 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008)
T_{min} = 0.424, T_{max} = 0.518
5549 measured reflections
1920 independent reflections
1253 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.137
S = 1.00
1920 reflections
122 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}
Absolute structure: Flack (1983), 801 Fiedel pairs
Flack parameter: −0.11 (13)

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work was supported by the National Natural Science Foundation of P. R. China (project No. 20971063 and 21101086) and the Natural Science Foundation of Shandong Province (Y2007B01).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2693).

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supplementary materials

Acta Cryst. (2012). E**68**, m169 [**doi:10.1107/S1600536811055176**]

catena-Poly[[trimethyltin(IV)]-μ-1,2,3-benzotriazol-1-ido-$\kappa^2N^1:N^3$]

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Comment

Several efforts have been made to prepare and study organotin compounds with nitrogen donor ligands not only because of their antitumor activity but also for the important role these compounds play in many biological processes (Pettinari *et al.*, 1996). Since then, only a few such complexes have been reported (Blaschette *et al.*, 1992; Wirth *et al.*, 1998; Berceanc *et al.*, 2002). As a contribution to this field, we report herein the crystal structure of the polymeric title compound.

In the title compound (Fig. 1), the Sn atom displays a distorted trigonal bipyramidal coordination geometry with the equatorial positions occupied by the carbon atoms of the three methyl groups and the apices by the N atoms of two symmetry-related benzotriazolato anion. The Sn—N bond distances are not remarkably different [Sn1—$N1^{i}$ = 2.356 (8); Sn1—N3 = 2.329 (8) Å; symmetry code: (i) 1/2-x, -1/2+y, 1/2-z], with an average value in agreement with those observed in related compounds. In the crystal structure, the benzotriazolato anions link adjacent $Sn(Me)_3$ units into zig-zag polymeric chains running parallel to the [011] and [0$\bar{1}$1] direction. Packing is stabilized only by van der Waals forces.

Experimental

The title compound was prepared by mixing trimethyltin (0.2 g, 1 mmol) and 1,2,3-benzotriazole (0.12 g, 1 mmol) in methanol (10 mL). The mixture was stirred for 7h, then the undissolved substance was filtered off. The title compound crystallized as red crystals after three weeks on slow evaporation of the solvent. Yield: 56%. Anal. Calc (%) for $C_{18}H_{26}N_6Sn_2$ (563.83): C, 38.31; H, 5.51. Found (%): C, 37.02; H, 5.36.

Refinement

All H atoms were placed in geometrically idealized positions and treated as riding on their parent atoms, with C—H = 0.93–0.96 Å and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C) for methyl H atoms.

Figures

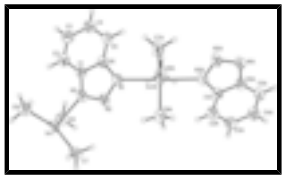


Fig. 1. The molecular structure of the title compound with 30% probability displacement ellipsoids. Symmetry code: (A) 1/2-x, 1/2+y, -1/2+z.

catena-Poly[[trimethyltin(IV)]-μ-1,2,3-benzotriazol-1-ido- $\kappa^2N^1:N^3$]

Crystal data

$[Sn(CH_3)_3(C_6H_4N_3)]$	$F(000) = 552$
$M_r = 281.93$	$D_x = 1.611$ Mg m^{-3}
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2c -2n	Cell parameters from 2591 reflections
$a = 14.8168$ (14) Å	$\theta = 2.3$–$28.1°$
$b = 10.6687$ (9) Å	$\mu = 2.16$ mm^{-1}
$c = 7.3518$ (7) Å	$T = 298$ K
$V = 1162.14$ (18) Å^3	Block, red
$Z = 4$	0.48 × 0.41 × 0.35 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	1920 independent reflections
Radiation source: fine-focus sealed tube	1253 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.031$
phi and ω scans	$\theta_{max} = 25.0°$, $\theta_{min} = 2.4°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008)	$h = -15\rightarrow17$
$T_{min} = 0.424$, $T_{max} = 0.518$	$k = -12\rightarrow12$
5549 measured reflections	$l = -7\rightarrow8$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.030$	$w = 1/[\sigma^2(F_o^2) + (0.0835P)^2 + 1.6416P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.137$	$(\Delta/\sigma)_{max} = 0.002$
$S = 1.00$	$\Delta\rho_{max} = 0.49$ e Å^{-3}
1920 reflections	$\Delta\rho_{min} = -0.49$ e Å^{-3}
122 parameters	Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
1 restraint	Extinction coefficient: 0.025 (2)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 801 Fiedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: −0.11 (13)

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

	x	*y*	*z*	U_{iso}*/U_{eq}

N1	0.1848 (6)	0.4850 (7)	0.0322 (11)	0.065 (2)
Sn1	0.25035 (3)	0.15544 (4)	0.3757 (6)	0.0479 (3)
C4	−0.0362 (7)	0.3651 (9)	−0.123 (2)	0.081 (3)
H4	−0.0862	0.3824	−0.1949	0.097*
C5	0.0335 (6)	0.4485 (8)	−0.120 (2)	0.075 (3)
H5	0.0331	0.5201	−0.1917	0.090*
N3	0.1867 (5)	0.3116 (7)	0.1954 (13)	0.067 (2)
C6	0.1055 (7)	0.4217 (8)	−0.0033 (13)	0.061 (2)
C7	0.3625 (7)	0.2679 (9)	0.4423 (16)	0.079 (3)
H7A	0.4164	0.2180	0.4382	0.118*
H7B	0.3549	0.3014	0.5625	0.118*
H7C	0.3673	0.3354	0.3565	0.118*
C1	0.1073 (7)	0.3123 (8)	0.0980 (14)	0.060 (2)
C9	0.1374 (7)	0.1572 (11)	0.555 (2)	0.102 (5)
H9A	0.1208	0.2423	0.5812	0.152*
H9B	0.1530	0.1152	0.6662	0.152*
H9C	0.0875	0.1149	0.4987	0.152*
N2	0.2332 (6)	0.4168 (8)	0.1502 (15)	0.067 (2)
C8	0.2505 (6)	0.0421 (12)	0.139 (2)	0.076 (4)
H8A	0.3055	0.0554	0.0726	0.115*
H8B	0.2000	0.0640	0.0637	0.115*
H8C	0.2462	−0.0445	0.1732	0.115*
C2	0.0372 (9)	0.2279 (11)	0.0931 (19)	0.085 (4)
H2	0.0384	0.1557	0.1639	0.102*
C3	−0.0351 (10)	0.2533 (11)	−0.020 (2)	0.088 (4)
H3	−0.0828	0.1969	−0.0286	0.106*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.074 (5)	0.059 (5)	0.062 (6)	0.000 (4)	0.001 (4)	0.014 (4)
Sn1	0.0570 (4)	0.0380 (4)	0.0489 (4)	0.0003 (2)	0.0018 (3)	0.0109 (3)
C4	0.083 (7)	0.084 (7)	0.075 (7)	0.001 (6)	−0.009 (9)	0.004 (8)
C5	0.082 (6)	0.068 (6)	0.075 (7)	0.001 (5)	0.004 (9)	0.020 (7)
N3	0.073 (5)	0.058 (5)	0.069 (6)	0.001 (4)	0.001 (5)	0.013 (4)
C6	0.073 (6)	0.057 (5)	0.054 (6)	0.005 (5)	0.003 (5)	0.001 (5)
C7	0.097 (7)	0.054 (6)	0.086 (8)	0.002 (5)	−0.018 (6)	0.012 (5)
C1	0.067 (6)	0.053 (5)	0.060 (7)	−0.005 (5)	−0.002 (5)	0.004 (5)
C9	0.083 (8)	0.103 (10)	0.119 (12)	0.018 (6)	0.022 (9)	0.042 (8)
N2	0.087 (6)	0.040 (4)	0.073 (7)	−0.001 (4)	−0.009 (5)	0.015 (4)
C8	0.096 (9)	0.053 (6)	0.080 (9)	−0.003 (4)	−0.020 (6)	−0.018 (5)
C2	0.087 (7)	0.073 (7)	0.094 (10)	−0.005 (6)	−0.002 (8)	0.018 (7)
C3	0.078 (7)	0.075 (8)	0.112 (11)	−0.010 (6)	−0.009 (8)	0.008 (7)

Geometric parameters (Å, °)

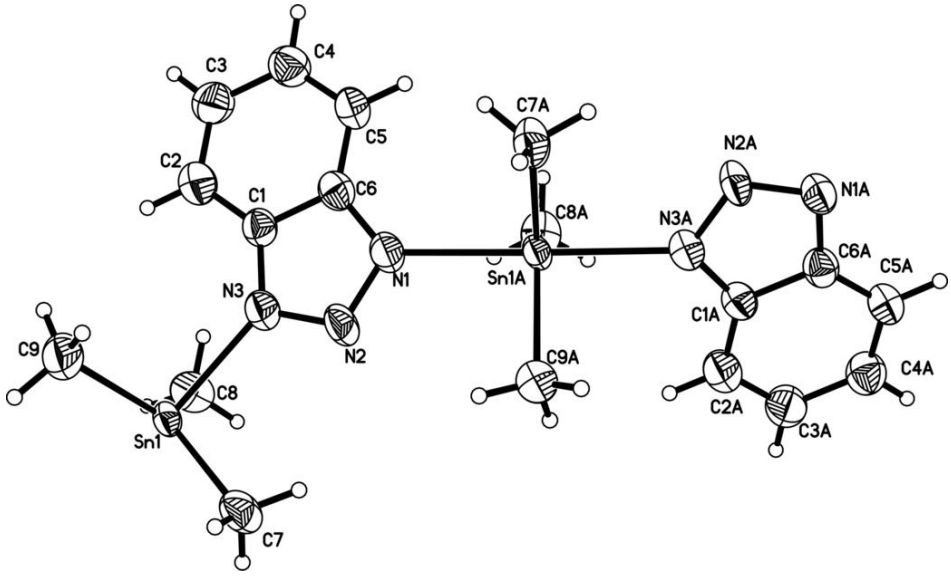
N1—N2	1.340 (11)	C6—C1	1.385 (12)
N1—C6	1.380 (12)	C7—H7A	0.9600

N1—Sn1^{i}	2.356 (8)	C7—H7B	0.9600
Sn1—C7	2.107 (10)	C7—H7C	0.9600
Sn1—C8	2.120 (13)	C1—C2	1.375 (13)
Sn1—C9	2.131 (13)	C9—H9A	0.9600
Sn1—N3	2.329 (8)	C9—H9B	0.9600
Sn1—N1^{ii}	2.356 (8)	C9—H9C	0.9600
C4—C5	1.364 (12)	C8—H8A	0.9600
C4—C3	1.411 (16)	C8—H8B	0.9600
C4—H4	0.9300	C8—H8C	0.9600
C5—C6	1.397 (15)	C2—C3	1.384 (19)
C5—H5	0.9300	C2—H2	0.9300
N3—N2	1.359 (11)	C3—H3	0.9300
N3—C1	1.376 (12)		
N2—N1—C6	108.2 (7)	H7A—C7—H7B	109.5
N2—N1—Sn1^{i}	121.1 (6)	Sn1—C7—H7C	109.5
C6—N1—Sn1^{i}	129.2 (6)	H7A—C7—H7C	109.5
C7—Sn1—C8	121.0 (5)	H7B—C7—H7C	109.5
C7—Sn1—C9	118.1 (6)	N3—C1—C2	131.0 (9)
C8—Sn1—C9	120.9 (5)	N3—C1—C6	107.5 (8)
C7—Sn1—N3	92.5 (3)	C2—C1—C6	121.5 (10)
C8—Sn1—N3	86.6 (5)	Sn1—C9—H9A	109.5
C9—Sn1—N3	91.6 (4)	Sn1—C9—H9B	109.5
C7—Sn1—N1^{ii}	90.3 (4)	H9A—C9—H9B	109.5
C8—Sn1—N1^{ii}	87.7 (5)	Sn1—C9—H9C	109.5
C9—Sn1—N1^{ii}	91.4 (4)	H9A—C9—H9C	109.5
N3—Sn1—N1^{ii}	174.3 (4)	H9B—C9—H9C	109.5
C5—C4—C3	122.3 (11)	N1—N2—N3	109.6 (8)
C5—C4—H4	118.9	Sn1—C8—H8A	109.5
C3—C4—H4	118.9	Sn1—C8—H8B	109.5
C4—C5—C6	117.1 (10)	H8A—C8—H8B	109.5
C4—C5—H5	121.5	Sn1—C8—H8C	109.5
C6—C5—H5	121.5	H8A—C8—H8C	109.5
N2—N3—C1	107.6 (8)	H8B—C8—H8C	109.5
N2—N3—Sn1	121.6 (6)	C3—C2—C1	118.2 (11)
C1—N3—Sn1	130.2 (6)	C3—C2—H2	120.9
N1—C6—C1	107.1 (9)	C1—C2—H2	120.9
N1—C6—C5	131.8 (9)	C2—C3—C4	119.7 (12)
C1—C6—C5	121.1 (9)	C2—C3—H3	120.1
Sn1—C7—H7A	109.5	C4—C3—H3	120.1
Sn1—C7—H7B	109.5		
C3—C4—C5—C6	−2.8 (17)	N2—N3—C1—C6	−1.6 (12)
C7—Sn1—N3—N2	10.1 (9)	Sn1—N3—C1—C6	−173.1 (7)
C8—Sn1—N3—N2	−110.8 (9)	N1—C6—C1—N3	0.9 (11)
C9—Sn1—N3—N2	128.3 (9)	C5—C6—C1—N3	178.9 (10)
C7—Sn1—N3—C1	−179.4 (10)	N1—C6—C1—C2	179.8 (11)
C8—Sn1—N3—C1	59.7 (9)	C5—C6—C1—C2	−2.2 (16)
C9—Sn1—N3—C1	−61.2 (10)	C6—N1—N2—N3	−1.2 (12)

N2—N1—C6—C1	0.1 (11)	$Sn1^{i}$—N1—N2—N3	−168.6 (7)
$Sn1^{i}$—N1—C6—C1	166.2 (7)	C1—N3—N2—N1	1.7 (12)
N2—N1—C6—C5	−177.5 (11)	Sn1—N3—N2—N1	174.1 (6)
$Sn1^{i}$—N1—C6—C5	−11.5 (16)	N3—C1—C2—C3	−179.8 (13)
C4—C5—C6—N1	−179.9 (10)	C6—C1—C2—C3	1.6 (19)
C4—C5—C6—C1	2.7 (15)	C1—C2—C3—C4	−2(2)
N2—N3—C1—C2	179.6 (12)	C5—C4—C3—C2	2(2)
Sn1—N3—C1—C2	8.2 (19)		

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

Fig. 1


C4
C3
C5
C2
C1
C6
N3
N1
N2
C9
C8
Sn1
C7
C7A
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C9A
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N1A
N3A
C6A
C5A
C1A
C4A
C2A
C3A