Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Dimethylbis(pyrazine-2-carboxylato-κ^2N^1,O)tin(IV)

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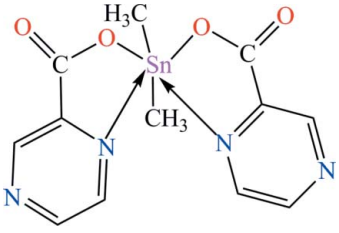
Received 4 October 2012; accepted 15 October 2012

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.020; wR factor = 0.051; data-to-parameter ratio = 16.6.

In the title compound, $[Sn(CH_3)_2(C_5H_3N_2O_2)_2]$, the Sn^{IV} atom is twice N,O-chelated by two pyrazine-2-carboxylate ligands. The distorted six-coordination is completed by two tin-bound methyl C atoms. The $C_2N_2O_2$ donor set defines a skewed trapezoidal–bipyramidal geometry. Intermolecular π–π interactions between the pyrazine rings [centroid–centroid distance = 3.8112 (13) Å] are observed.

Related literature

For background to organotin compounds, see: Dakternieks *et al.* (2003); Tiekink (1991); Yin *et al.* (2005).



Experimental

Crystal data

$[Sn(CH_3)_2(C_5H_3N_2O_2)_2]$
M_r = 394.95
Monoclinic, $P2_1/c$
a = 9.2887 (6) Å
b = 12.3253 (7) Å
c = 12.6596 (7) Å
β = 103.738 (1)°
V = 1407.88 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.84 mm^{-1}
T = 295 K
0.40 × 0.40 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.527, T_{max} = 0.710
8657 measured reflections
3193 independent reflections
2892 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.051
S = 1.06
3193 reflections
192 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sn1—C1	2.097 (2)	Sn1—O3	2.1238 (15)
Sn1—C2	2.095 (2)	Sn1—N1	2.6646 (18)
Sn1—O1	2.1506 (16)	Sn1—N3	2.5107 (18)

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: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank Shahid Beheshti University for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2594).

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supporting information

Acta Cryst. (2012). E**68**, m1384 [doi:10.1107/S160053681204295X]

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S1. Comment

The reaction of appropriate amount of dimethyltin dichloride and pyrazine-2-carboxylic acid in dry methanol provided the title compound in good yield. The six-coordinated geometry around the Sn^{IV} atom is better described as skew-trapezoidal bipyramidal (Fig. 1, Table 1). Intermolecular π–π interactions between the pyrazine rings [centroid–centroid distance = 3.8112 (13) Å] stabilize the structure.

S2. Experimental

Dimethyltin dichloride (0.22 g, 1 mmol) was treated with sodium methoxide (0.1 g, 2 mmol) in methanol (10 ml) to produce dimethyltin dimethoxide and sodium chloride. The sodium chloride precipitate was removed by filtration and then pyrazine-2-carboxylic acid (0.248 g, 2 mmol) in methanol (20 ml) was added to the filtrate. The solution was refluxed for 3 h. Evaporation of the solvent yielded a white solid, which was purified by recrystallization from methanol (yield: 70%. m.p.: 118–120°C).

S3. Refinement

H atoms were placed in calculated positions and refined as riding atoms, with C–H = 0.93 (CH) and 0.96 (CH_3) Å and with U_{iso}(H) = 1.2(1.5 for methyl)U_{eq}(C). Omitted reflections owing to bad disagreement were (-9 10 6), (-6 13 3), (8 0 4), (2 0 8) and (-1 8 6).

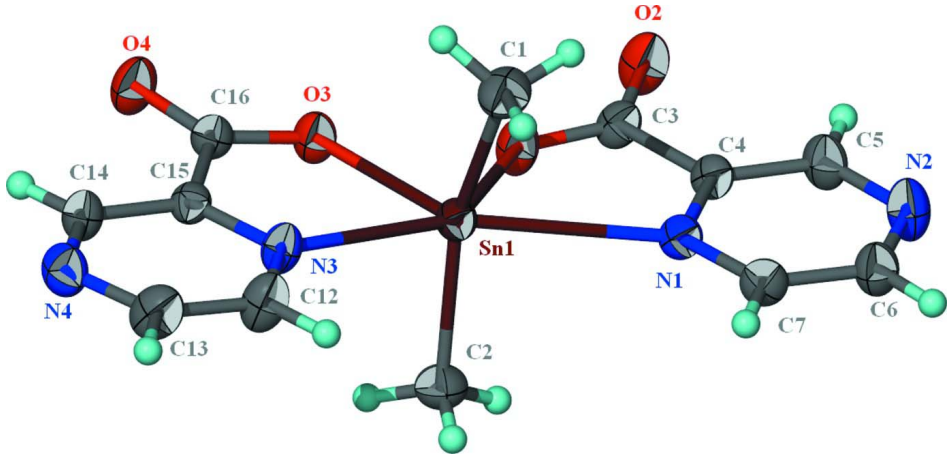

Figure 1

Molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

Dimethylbis(pyrazine-2-carboxylato-κ^2N^1,O)tin(IV)

Crystal data

$[Sn(CH_3)_2(C_5H_3N_2O_2)_2]$
$M_r = 394.95$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.2887$ (6) Å
$b = 12.3253$ (7) Å
$c = 12.6596$ (7) Å
$\beta = 103.738$ (1)°
$V = 1407.88$ (14) Å^3
$Z = 4$
$F(000) = 776$
$D_x = 1.863$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5890 reflections
$\theta = 2.3$–$28.3°$
$\mu = 1.84$ mm^{-1}
$T = 295$ K
Prism, colorless
0.40 × 0.40 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.527$, $T_{max} = 0.710$
8657 measured reflections
3193 independent reflections
2892 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
$h = -12 \rightarrow 11$
$k = -16 \rightarrow 13$
$l = -15 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.020$
$wR(F^2) = 0.051$
$S = 1.06$
3193 reflections
192 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0201P)^2 + 0.7349P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.47$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.826212 (14)	0.699389 (11)	0.602141 (11)	0.02943 (6)
O1	0.87907 (17)	0.71196 (14)	0.44616 (13)	0.0415 (4)
O2	0.99121 (19)	0.78275 (16)	0.32619 (13)	0.0493 (4)
O3	0.62830 (16)	0.65997 (14)	0.48535 (12)	0.0374 (3)
O4	0.39196 (17)	0.61066 (15)	0.43503 (13)	0.0469 (4)
N1	1.09601 (19)	0.77904 (14)	0.61292 (14)	0.0320 (4)
N2	1.3488 (2)	0.87890 (18)	0.57415 (17)	0.0478 (5)
N3	0.62453 (19)	0.65022 (15)	0.69497 (14)	0.0340 (4)
N4	0.3759 (2)	0.57674 (16)	0.76062 (16)	0.0421 (4)
C1	0.7815 (3)	0.86219 (19)	0.6305 (2)	0.0466 (6)
H1A	0.8346	0.9084	0.5918	0.070*
H1B	0.8123	0.8772	0.7070	0.070*
H1C	0.6770	0.8755	0.6057	0.070*

C2	0.9233 (3)	0.54697 (19)	0.6433 (2)	0.0444 (5)
H2A	1.0075	0.5391	0.6123	0.067*
H2B	0.8523	0.4912	0.6155	0.067*
H2C	0.9546	0.5408	0.7210	0.067*
C3	0.9857 (2)	0.76167 (19)	0.41998 (17)	0.0346 (4)
C4	1.1116 (2)	0.79754 (16)	0.51203 (17)	0.0302 (4)
C5	1.2359 (3)	0.8484 (2)	0.49323 (19)	0.0405 (5)
H5	1.2409	0.8618	0.4219	0.049*
C6	1.3319 (3)	0.86057 (19)	0.67419 (19)	0.0417 (5)
H6	1.4074	0.8812	0.7331	0.050*
C7	1.2068 (3)	0.81211 (17)	0.69396 (18)	0.0361 (5)
H7	1.1996	0.8023	0.7654	0.043*
C12	0.6207 (3)	0.6469 (2)	0.79961 (18)	0.0445 (6)
H12	0.7030	0.6696	0.8523	0.053*
C13	0.4970 (3)	0.6103 (2)	0.83094 (19)	0.0449 (6)
H13	0.4986	0.6092	0.9047	0.054*
C14	0.3798 (2)	0.58104 (18)	0.65644 (18)	0.0367 (5)
H14	0.2974	0.5577	0.6042	0.044*
C15	0.5024 (2)	0.61905 (16)	0.62266 (16)	0.0295 (4)
C16	0.5045 (2)	0.62962 (16)	0.50495 (17)	0.0321 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.02845 (8)	0.03258 (9)	0.02919 (9)	0.00030 (5)	0.01068 (6)	0.00025 (5)
O1	0.0333 (8)	0.0637 (11)	0.0291 (8)	−0.0101 (7)	0.0106 (6)	−0.0007 (7)
O2	0.0415 (9)	0.0830 (13)	0.0266 (8)	−0.0074 (8)	0.0144 (7)	0.0015 (8)
O3	0.0337 (8)	0.0518 (9)	0.0280 (7)	−0.0071 (7)	0.0097 (6)	0.0015 (7)
O4	0.0346 (8)	0.0667 (11)	0.0359 (8)	−0.0095 (8)	0.0012 (7)	−0.0012 (8)
N1	0.0310 (9)	0.0379 (9)	0.0296 (9)	0.0011 (7)	0.0123 (7)	0.0020 (7)
N2	0.0421 (11)	0.0589 (13)	0.0449 (11)	−0.0164 (9)	0.0151 (9)	−0.0052 (10)
N3	0.0278 (8)	0.0442 (10)	0.0309 (9)	−0.0032 (7)	0.0088 (7)	−0.0047 (8)
N4	0.0380 (10)	0.0471 (11)	0.0464 (11)	−0.0019 (8)	0.0203 (9)	0.0023 (9)
C1	0.0429 (13)	0.0383 (12)	0.0571 (15)	0.0043 (10)	0.0089 (11)	−0.0073 (11)
C2	0.0437 (13)	0.0380 (12)	0.0511 (14)	0.0060 (10)	0.0104 (11)	0.0047 (10)
C3	0.0303 (10)	0.0456 (12)	0.0303 (10)	0.0039 (9)	0.0119 (8)	−0.0010 (9)
C4	0.0287 (10)	0.0363 (10)	0.0289 (10)	0.0026 (8)	0.0134 (8)	−0.0002 (8)
C5	0.0397 (12)	0.0510 (13)	0.0353 (11)	−0.0075 (10)	0.0175 (9)	0.0000 (10)
C6	0.0394 (12)	0.0449 (13)	0.0404 (12)	−0.0090 (10)	0.0082 (10)	−0.0043 (10)
C7	0.0402 (12)	0.0396 (11)	0.0296 (11)	0.0002 (9)	0.0106 (9)	−0.0006 (8)
C12	0.0348 (11)	0.0687 (16)	0.0308 (11)	−0.0037 (11)	0.0093 (9)	−0.0065 (11)
C13	0.0424 (12)	0.0627 (15)	0.0338 (11)	0.0054 (11)	0.0171 (10)	0.0010 (11)
C14	0.0301 (10)	0.0415 (12)	0.0399 (12)	−0.0040 (9)	0.0109 (9)	−0.0025 (9)
C15	0.0276 (9)	0.0286 (10)	0.0333 (10)	0.0016 (7)	0.0091 (8)	−0.0016 (8)
C16	0.0305 (10)	0.0330 (10)	0.0328 (10)	−0.0004 (8)	0.0079 (8)	−0.0006 (8)

Geometric parameters (Å, º)

Sn1—C1	2.097 (2)	C1—H1A	0.9600
Sn1—C2	2.095 (2)	C1—H1B	0.9600
Sn1—O1	2.1506 (16)	C1—H1C	0.9600
Sn1—O3	2.1238 (15)	C2—H2A	0.9600
Sn1—N1	2.6646 (18)	C2—H2B	0.9600
Sn1—N3	2.5107 (18)	C2—H2C	0.9600
O1—C3	1.274 (3)	C3—C4	1.508 (3)
O2—C3	1.228 (3)	C4—C5	1.383 (3)
O3—C16	1.288 (3)	C5—H5	0.9300
O4—C16	1.221 (2)	C6—C7	1.382 (3)
N1—C7	1.332 (3)	C6—H6	0.9300
N1—C4	1.339 (3)	C7—H7	0.9300
N2—C6	1.332 (3)	C12—C13	1.378 (3)
N2—C5	1.334 (3)	C12—H12	0.9300
N3—C12	1.334 (3)	C13—H13	0.9300
N3—C15	1.334 (3)	C14—C15	1.389 (3)
N4—C13	1.324 (3)	C14—H14	0.9300
N4—C14	1.329 (3)	C15—C16	1.501 (3)
C2—Sn1—C1	154.98 (10)	Sn1—C2—H2C	109.5
C2—Sn1—O3	102.62 (8)	H2A—C2—H2C	109.5
C1—Sn1—O3	99.44 (8)	H2B—C2—H2C	109.5
C2—Sn1—O1	96.58 (8)	O2—C3—O1	124.5 (2)
C1—Sn1—O1	100.72 (9)	O2—C3—C4	118.9 (2)
O3—Sn1—O1	74.09 (6)	O1—C3—C4	116.63 (18)
C2—Sn1—N3	89.54 (8)	N1—C4—C5	121.7 (2)
C1—Sn1—N3	87.17 (9)	N1—C4—C3	116.59 (18)
O3—Sn1—N3	69.63 (6)	C5—C4—C3	121.71 (19)
O1—Sn1—N3	143.67 (6)	N2—C5—C4	122.1 (2)
C2—Sn1—N1	88.49 (8)	N2—C5—H5	118.9
C1—Sn1—N1	82.01 (8)	C4—C5—H5	118.9
O3—Sn1—N1	140.17 (5)	N2—C6—C7	122.7 (2)
O1—Sn1—N1	66.64 (6)	N2—C6—H6	118.7
N3—Sn1—N1	149.56 (5)	C7—C6—H6	118.7
C3—O1—Sn1	129.40 (14)	N1—C7—C6	121.4 (2)
C16—O3—Sn1	126.66 (13)	N1—C7—H7	119.3
C7—N1—C4	116.35 (18)	C6—C7—H7	119.3
C7—N1—Sn1	134.17 (14)	N3—C12—C13	121.1 (2)
C4—N1—Sn1	109.12 (13)	N3—C12—H12	119.5
C6—N2—C5	115.7 (2)	C13—C12—H12	119.5
C12—N3—C15	116.99 (19)	N4—C13—C12	122.8 (2)
C12—N3—Sn1	132.12 (15)	N4—C13—H13	118.6
C15—N3—Sn1	110.85 (13)	C12—C13—H13	118.6
C13—N4—C14	115.86 (19)	N4—C14—C15	122.4 (2)
Sn1—C1—H1A	109.5	N4—C14—H14	118.8
Sn1—C1—H1B	109.5	C15—C14—H14	118.8

H1A—C1—H1B	109.5	N3—C15—C14	120.76 (19)
Sn1—C1—H1C	109.5	N3—C15—C16	116.52 (18)
H1A—C1—H1C	109.5	C14—C15—C16	122.70 (18)
H1B—C1—H1C	109.5	O4—C16—O3	124.5 (2)
Sn1—C2—H2A	109.5	O4—C16—C15	119.47 (19)
Sn1—C2—H2B	109.5	O3—C16—C15	116.07 (17)
H2A—C2—H2B	109.5		

C2—Sn1—O1—C3	−98.1 (2)	C7—N1—C4—C5	−0.1 (3)
C1—Sn1—O1—C3	63.8 (2)	Sn1—N1—C4—C5	173.91 (17)
O3—Sn1—O1—C3	160.6 (2)	C7—N1—C4—C3	−179.20 (18)
N3—Sn1—O1—C3	163.69 (17)	Sn1—N1—C4—C3	−5.2 (2)
N1—Sn1—O1—C3	−12.59 (18)	O2—C3—C4—N1	175.7 (2)
C2—Sn1—O3—C16	83.58 (19)	O1—C3—C4—N1	−3.5 (3)
C1—Sn1—O3—C16	−84.53 (19)	O2—C3—C4—C5	−3.4 (3)
O1—Sn1—O3—C16	176.92 (19)	O1—C3—C4—C5	177.4 (2)
N3—Sn1—O3—C16	−1.15 (17)	C6—N2—C5—C4	−2.2 (4)
N1—Sn1—O3—C16	−173.35 (15)	N1—C4—C5—N2	2.0 (4)
C2—Sn1—N1—C7	−81.4 (2)	C3—C4—C5—N2	−178.9 (2)
C1—Sn1—N1—C7	75.4 (2)	C5—N2—C6—C7	0.7 (4)
O3—Sn1—N1—C7	170.55 (17)	C4—N1—C7—C6	−1.4 (3)
O1—Sn1—N1—C7	−179.2 (2)	Sn1—N1—C7—C6	−173.53 (16)
N3—Sn1—N1—C7	5.1 (3)	N2—C6—C7—N1	1.2 (4)
C2—Sn1—N1—C4	106.05 (15)	C15—N3—C12—C13	1.5 (4)
C1—Sn1—N1—C4	−97.16 (15)	Sn1—N3—C12—C13	−175.99 (18)
O3—Sn1—N1—C4	−1.98 (18)	C14—N4—C13—C12	−0.5 (4)
O1—Sn1—N1—C4	8.22 (13)	N3—C12—C13—N4	0.0 (4)
N3—Sn1—N1—C4	−167.44 (13)	C13—N4—C14—C15	−0.5 (3)
C2—Sn1—N3—C12	77.7 (2)	C12—N3—C15—C14	−2.4 (3)
C1—Sn1—N3—C12	−77.5 (2)	Sn1—N3—C15—C14	175.58 (16)
O3—Sn1—N3—C12	−178.7 (2)	C12—N3—C15—C16	176.3 (2)
O1—Sn1—N3—C12	178.2 (2)	Sn1—N3—C15—C16	−5.6 (2)
N1—Sn1—N3—C12	−8.5 (3)	N4—C14—C15—N3	2.0 (3)
C2—Sn1—N3—C15	−99.93 (15)	N4—C14—C15—C16	−176.7 (2)
C1—Sn1—N3—C15	104.88 (15)	Sn1—O3—C16—O4	177.83 (17)
O3—Sn1—N3—C15	3.72 (13)	Sn1—O3—C16—C15	−1.4 (3)
O1—Sn1—N3—C15	0.6 (2)	N3—C15—C16—O4	−174.2 (2)
N1—Sn1—N3—C15	173.84 (12)	C14—C15—C16—O4	4.6 (3)
Sn1—O1—C3—O2	−164.70 (18)	N3—C15—C16—O3	5.1 (3)
Sn1—O1—C3—C4	14.5 (3)	C14—C15—C16—O3	−176.11 (19)