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Octamethyl-1κ^2C,2κ^2C,3κ^2C,4κ^2C-bis(μ_2-2-methylpyrazine-5-carboxylato)-1:2κ^2O:O;3:4κ^2O:O-bis(2-methylpyrazine-5-carboxylato)-1κO,4κO-di-μ_3-oxido-1:2:3κ^3O:O:O;2:3:4κ^3O:O:O-tetratin(IV) hexahydrate

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The title compound, $[Sn_4(CH_3)_8(C_6H_5N_2O_2)_4O_2]\cdot 6H_2O$, is a hydrated cluster containing four Sn atoms, built up by inversion symmetry around the central Sn_2O_2 ring. The Sn-atom coordination geometry might be regarded as very distorted SnO_3C_2 trigonal–bipyramidal or possibly as grossly distorted SnO_3C_2N octahedral. All the cluster non-H atoms, with the exception of the Sn-bonded methyl groups, lie on a mirror plane. Two of the water-molecule O atoms have *m* site symmetry; the other occupies a twofold rotation axis.

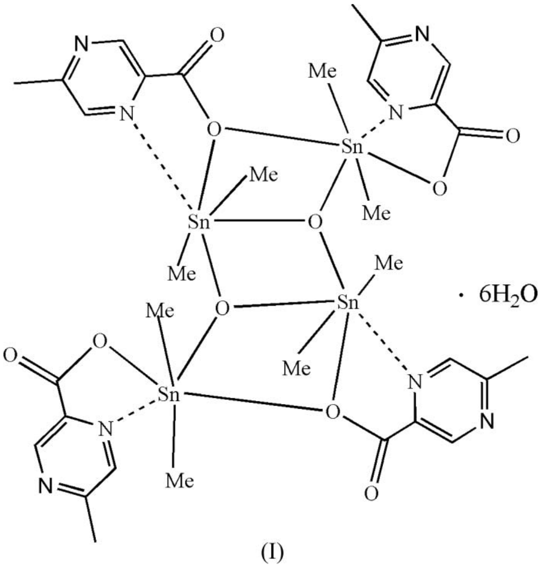
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.011 Å
R factor = 0.030
wR factor = 0.079
Data-to-parameter ratio = 14.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The title compound, $C_{32}H_{44}N_8O_{10}Sn_4\cdot 6H_2O$, (I) (Fig. 1), is a hydrated cluster containing four Sn atoms. The molecule, with a central Sn_2O_2 core, is centrosymmetric. The three-coordinate, μ_3-bridging atom O5 in the Sn_2O_2 ring is also attached to an Me_2SnO_2 unit. Furthermore, O3 coordinates to both Sn1 and Sn2. All the cluster non-H atoms, with the exception of the Sn-bonded methyl groups, lie on a mirror plane. Of the water molecules, O6 and O7 lie on a mirror plane, and O8 lies on a twofold rotation axis.



(I)

The Sn-atom geomety in (I) might be regarded as extremely distorted trigonal–bipyramidal (Table 1) with the C atoms in equatorial positions. For Sn1, the distortion is so large that the C13—Sn1—C13^{i} (see Table 1 for symmetry codes) bond angle of 147.8 (3)° is only slightly smaller than the nominal axial O1—Sn1—O3^{ii} bond angle of 149.44 (16)°.

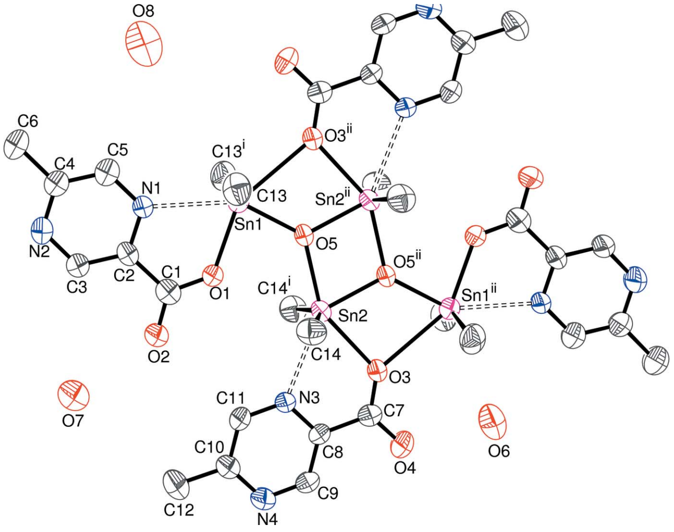


Figure 1
The molecular structure of (I) with 30% displacement ellipsoids (H atoms omitted for clarity); the short Sn···N contacts are indicated by double-dashed lines. Symmetry codes as in Table 1.

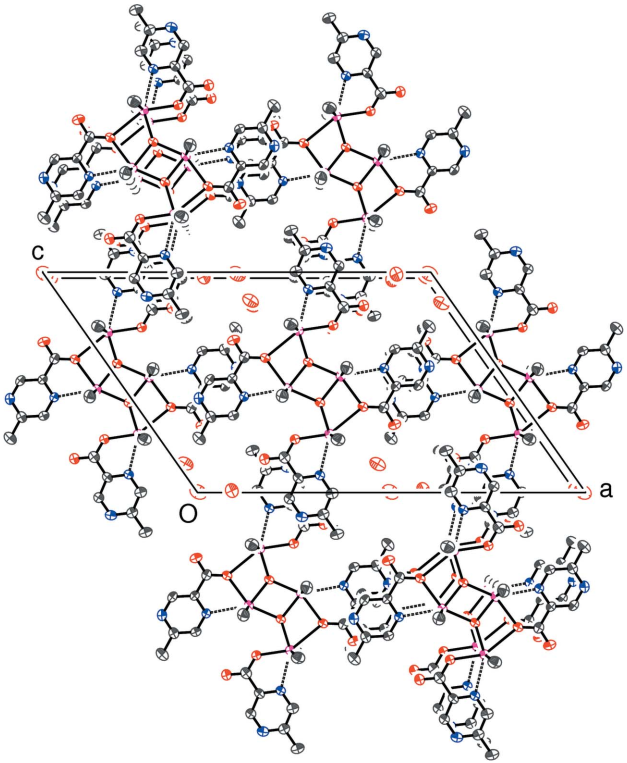


Figure 2
The packing of (I), viewed down [010], with H atoms omitted for clarity; Sn···N contacts are indicated by dashed lines.

The widening of the C—Sn—C equatorial bonds appears to be correlated with short Sn···N contacts arising from N atoms in the attached pyrazine rings. If the short Sn···N contacts in (I) are regarded as bonds (Table 1), then grossly distorted SnO_3C_2N octahedra result for both Sn1 and Sn2. The sum of the van der Waals radii for Sn and N is 4.0 Å (Vollano *et al.*, 1984).

The crystal packing results in [010] channels occupied by the non-coordinating water molecules (Fig. 2). Probable hydrogen bonds (Table 2) involving the water molecules are present. Compound (I) complements other tin clusters with Sn_2O_2 cores (*e.g.* Puff *et al.*, 1983; Mohamed *et al.*, 2004).

Experimental

A mixture of dimethyltin(IV) dichloride (2.0 mmol, 0.439 g), 2-methylpyrazine-5-carboxylic acid (2.0 mmol, 0.276 g) and sodium ethoxide (2.0 mmol, 0.136 g) in ethanol (80 ml) was heated under reflux for 24 h at 326 K. The resulting clear solution was evaporated under vacuum. The product was crystallized from methanol to give blocks of (I). Yield 0.558 g, 78%, m.p. 396 K. Analysis, calculated for $C_{32}H_{56}N_8O_{16}Sn_4$: C 29.94, N 8.73, H, 4.40%; found: C 29.98, N 8.82, H 4.59%.

Crystal data

$[Sn_4(CH_3)_8(C_6H_5N_2O_2)_4O_2]\cdot 6H_2O$
$M_r = 1283.61$
Monoclinic, $C2/m$
$a = 23.735$ (6) Å
$b = 7.543$ (2) Å
$c = 16.468$ (4) Å
$\beta = 125.137$ (2)°
$V = 2411.1$ (11) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 2.12$ mm^{-1}
$T = 298$ (2) K
0.47 × 0.43 × 0.38 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{\min} = 0.436$, $T_{\max} = 0.500$ (expected range = 0.390–0.447)
6744 measured reflections
2541 independent reflections
1920 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.053$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.079$
$S = 1.09$
2541 reflections
176 parameters
H-atom parameters constrained
$\Delta\rho_{\max} = 1.01$ e Å^{-3}
$\Delta\rho_{\min} = -0.64$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Sn1—O5	2.020 (4)	Sn2—O5^{ii}	2.034 (4)
Sn1—C13^{i}	2.093 (5)	Sn2—C14^{i}	2.102 (5)
Sn1—C13	2.093 (5)	Sn2—C14	2.102 (5)
Sn1—O1	2.136 (4)	Sn2—O5	2.154 (4)
Sn1—N1	2.589 (5)	Sn2—O3	2.312 (4)
Sn1—O3^{ii}	2.642 (4)	Sn2—N3	2.712 (5)

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H1···O4	0.92	1.72	2.638 (8)	177
O6—H2···O8^{iii}	0.90	1.85	2.750 (6)	179
O7—H3···O2	0.90	1.90	2.798 (7)	180
O7—H4···O8^{iv}	0.90	1.87	2.774 (6)	180
O8—H5···O6^{v}	0.90	1.85	2.750 (6)	179
O8—H6···O7^{vi}	0.90	1.87	2.774 (6)	180

Symmetry codes: (iii) $x, y - 1, z + 1$; (iv) $-x + \frac{1}{2}, -y + \frac{1}{2}, -z$; (v) $x, y + 1, z - 1$; (vi) $x + \frac{1}{2}, y + \frac{1}{2}, z$.

Acta Cryst. (2007). E**63**, m1246–m1248 Li *et al.* • $[Sn_4(CH_3)_8(C_6H_5N_2O_2)_4O_2]\cdot 6H_2O$ **m1247**

The H atoms of the water molecules (O6, O7 and O8) could not be located in difference maps and were positioned geometrically (O—H = 0.90–0.92 Å) to generate a plausible hydrogen-bonding scheme with nearby cluster O atoms or other water O atoms; they were refined as riding atoms with $U_{iso}(H) = 1.2U_{eq}(O)$. Crystallographic symmetry seems to require that one H atom is disordered for each of O6 and O7 and that both H atoms are disordered for O8. The hydrogen-bonding scheme described here must be regarded as tentative. The C-bound H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C). The C13 and C14 methyl groups were allowed to rotate but not to tip, to best fit the electron density. The largest residual electron density peak is 0.74 Å from O4.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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