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Tetrakis(iodomethyl)stannane

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(Sn–C) = 0.008 Å
R factor = 0.038
wR factor = 0.105
Data-to-parameter ratio = 56.7

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

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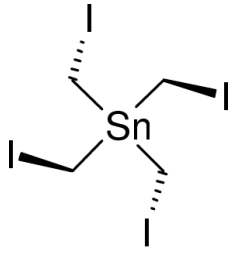
The structure of the title compound, $[Sn(CH_2I)_4]$, consists of Sn situated on a crystallographic fourfold rotatory inversion axis, with pendant iodomethyl groups whose atoms are in general positions. In the molecule, with overall crystallographically imposed S_4 molecular symmetry, there is little, if any, distortion of the tetrahedral environment of Sn, but the bulk of I leads to opening up of the Sn—C—I angle to 112.4 (3)°.

Comment

The asymmetric unit of the title compound, (I), consists of Sn in the 2*b* special positions of the space group $P\bar{4}2_1c$ along with, in the 8*e* general positions, C, I and two H atoms of a single representative iodomethyl group. As a consequence, relatively high S_4 symmetry is imposed upon the molecule as a whole, which is shown in Fig. 1, and results in the very compact presentation of symmetry-unique bond lengths and angles in Table 1. The bond distances are much as would be expected for a molecule of this type. The bond-angle data show that there is no real distortion of the tetrahedral coordination of Sn. However, the Sn1—C1—I1 angle of 112.4 (3)° is clearly attributable to the physical bulk of the I atom.



(I)

Experimental

Compound (I), prepared as described by Burnett *et al.* (1998) (m.p. 348–349 K) and recrystallized from $CHCl_3$, provided crystals suitable for analysis.

Crystal data

$[Sn(CH_2I)_4]$
M_r = 682.40
Tetragonal, $P\bar{4}2_1c$
a = 9.4019 (5) Å
c = 7.4051 (4) Å
V = 654.58 (6) Å^3
Z = 2
D_x = 3.462 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3436 reflections
θ = 3.1–30.5°
μ = 11.33 mm^{-1}
T = 298 (2) K
Block, colourless
0.40 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	1191 independent reflections
φ and ω scans	1044 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)	$R_{int} = 0.030$
$T_{min} = 0.416$, $T_{max} = 0.928$	$\theta_{max} = 32.6^\circ$
6440 measured reflections	$h = -12 \rightarrow 14$
	$k = -14 \rightarrow 13$
	$l = -11 \rightarrow 10$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0512P)^2 + 1.6332P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.038$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.105$	$\Delta\rho_{max} = 0.82$ e Å^{-3}
$S = 1.08$	$\Delta\rho_{min} = -1.58$ e Å^{-3}
1191 reflections	Absolute structure: (Flack, 1983)
21 parameters	Flack parameter = 0.06 (18)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Sn1—C1	2.114 (8)	I1—C1	2.135 (8)
C1—Sn1—C1^{i}	109.1 (5)	Sn1—C1—I1	112.4 (3)
C1—Sn1—C1^{ii}	109.7 (3)		

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

H atoms were placed in calculated positions, with C—H = 0.97 Å, and refined with a riding model, with $U_{iso} = 1.2U_{eq}$(C). The absolute structure was determined on the basis of 492 Friedel pairs.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

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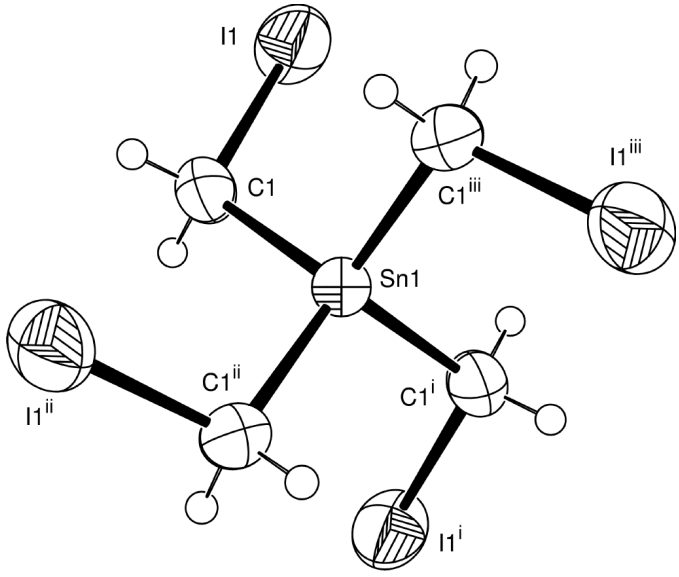

Figure 1
The molecule of (I), showing the labelling scheme. Non-H atoms are shown as 50% ellipsoids and H atoms as small circles. The view is down *c* of the tetragonal cell. [Symmetry codes: (i) $1-x, 1-y, z$; (ii) $1-y, x, 2-z$; (iii) $y, 1-x, 2-z$.]

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