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Tetrakis(2-methyl-2-phenylpropyl)-stannane at 150 K

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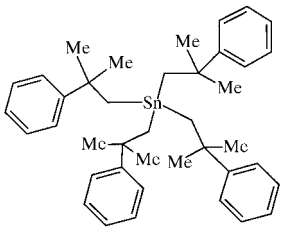
The structure of the title compound, tetrakis(2-methyl-2-phenylpropyl)stannane, $(PhCMe_2CH_2)_4Sn$, has been determined at 293 K by Reuter & Pawlak (1998). This present determination was carried out at 150 K and as a result gives cell, coordinate and displacement parameters with much reduced s.u.'s. As is pointed out in the the above paper, the bonds and angles are similar to those in related Sn compounds although it is worth emphasizing that there are no intra- or intermolecular ring–ring interactions but that there are a numberof C—H...Cg(π-ring) interactions at the 3.0 Å level.

Comment

Examination of the structure (I) with *PLATON* (Spek, 1999) showed that there were no solvent-accessible voids in the crystal lattice.



(I)

Experimental

Tetrakis(2-methyl-2-phenylpropyl)stannane was prepared from the Gringnard reagent, from $PhCMe_2CH_2Cl$ and Mg in Et_2O and $SnCl_4$ in benzene. It was recrystallized as colourless crystals from petroleum ether (60–80°C) and had a melting point of 94–96°C.

Crystal data

$[Sn(C_{10}H_{13})_4]$	D_x = 1.255 Mg m^{-3}
M_r = 651.51	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 7414 reflections
a = 13.9224 (4) Å	θ = 1.51–27.48°
b = 9.9590 (2) Å	μ = 0.766 mm^{-1}
c = 25.6952 (6) Å	T = 150.0 (1) K
β = 104.5178 (14)°	Lath, colourless
V = 3448.96 (15) Å^3	0.300 × 0.100 × 0.025 mm
Z = 4	

Data collection

KappaCCD diffractometer	7414 independent reflections
φ s and ω scans with κ offset scans	5147 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SORTAV; Blessing, 1995, 1997)	R_{int} = 0.064
T_{min} = 0.927, T_{max} = 0.973	θ_{max} = 27.48°
24777 measured reflections	$h = -17 \rightarrow 17$
	$k = -12 \rightarrow 12$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.038	$w = 1/[\sigma^2(F_o^2) + (0.0265P)^2 + 1.4792P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.088	$(\Delta/\sigma)_{max}$ = 0.004
S = 0.989	$\Delta\rho_{max}$ = 0.828 e Å^{-3}
7414 reflections	$\Delta\rho_{min}$ = −0.737 e Å^{-3}
378 parameters	

Molecule (1) crystallized in the monoclinic system; space group $P2_1/c$ from the systematic absences. H atoms were treated as riding atoms with C—H 0.90–0.98 Å.

Data collection: KappaCCD server software (Nonius, 1997); cell refinement: DENZO (Otwinowski & Minor, 1997); data reduction: DENZO (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL*97 and *WordPerfect* macro PRPKAPPA (Ferguson, 1999).

X-ray data were collected at the EPSRC, X-ray Crystallographic Service, University of Southampton using a Enraf–Nonius KappaCCD diffractometer. The authors thank the staff for all their help and advice.

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