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Chlorotris(2-methyl-2-phenylpropyl)-tin(IV) at 150 K

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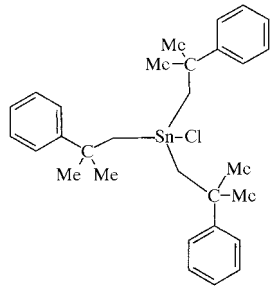
The structure of the title compound, $[SnCl(C_{10}H_{13})_3]$, (I), was originally determined at room temperature and published without atomic coordinates by Schomburg, Link, Linoh & Tacke [*J. Organomet. Chem.* (1988), **339**, 69–80]. We report



(I)

here the structural determination at 150 K. The cell dimension shows a contraction from 22.5251 (8) to 22.3858 (4) Å, as expected.

Experimental

The title compound was prepared from the corresponding oxide and HCl. Crystals were obtained by the slow evaporation of a $CHCl_3$ solution [m.p. 389–390 K; literature value: m.p. 389.5–390.5 K (Zimmer *et al.*, 1966)].

Crystal data

$[SnCl(C_{10}H_{13})_3]$
M_r = 553.75
Cubic, $I\bar{4}3d$
a = 22.3858 (4) Å
V = 11218.1 (3) Å^3
Z = 16
D_x = 1.311 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2073 reflections
θ = 3.40–27.40°
μ = 1.021 mm^{-1}
T = 150.0 (1) K
Block, colourless
0.38 × 0.25 × 0.13 mm

Data collection

KappaCCD diffractometer
φ and ω scans with κ offsets
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995, 1997)
T_{min} = 0.701, T_{max} = 0.883
11 754 measured reflections
2073 independent reflections
1602 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 27.40°
$h = -9 \rightarrow 29$
$k = -23 \rightarrow 29$
$l = -24 \rightarrow 26$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.123
S = 1.043
2073 reflections
99 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0747P)^2 + 4.8319P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}
Absolute structure: Flack (1983), 927 Friedel pairs
Flack parameter = −0.06 (6)

Molecule (I) crystallized in the cubic system; space group $I\bar{4}3d$ from the systematic absences. H atoms were treated as riding atoms with C—H = 0.95–0.98 Å. Examination of the structure with *PLATON* (Spek, 2000) showed that there were no solvent-accessible voids in the crystal lattice.

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); 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 an Enraf–Nonius KappaCCD diffractometer. The authors thank the staff for all their help and advice.

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