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Tetrakis(2,4,5-trichlorophenyl)stannane

Nadim S. Shaikh,[a] Sean Parkin[b] and Hans-Joachim Lehmler[c]*

[a]Leibniz-Institut für Katalyse, Albert-Einstein-Strasse 29a, D-18059 Rostock, Germany, [b]University of Kentucky, Department of Chemistry, Lexington, KY 40506-0055, USA, and [c]The University of Iowa, Department of Occupational and Environmental Health, 100 Oakdale Campus, 221 IREH, Iowa City, IA 52242-5000, USA

Correspondence e-mail:
hans-joachim-lehmler@uiowa.edu

Key indicators

Single-crystal X-ray study
T = 90 K
Mean *σ*(C–C) = 0.004 Å
R factor = 0.024
wR factor = 0.059
Data-to-parameter ratio = 15.0

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

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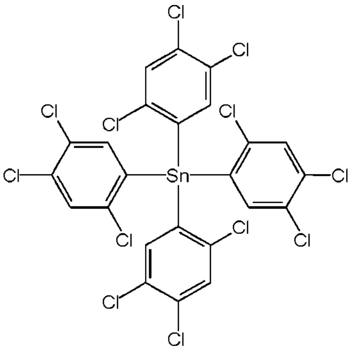
The molecule of the title compound, $[Sn(C_6H_2Cl_3)_4]$, occupies a general position in the crystal structure, but shows an approximate $\overline{4}$ molecular symmetry.

Comment

Tetraarylstannanes are an important class of organotin compounds that are of interest for both technical and biomedical applications (Pellerito *et al.*, 2006; Gielen, 2002). Therefore, new and improved approaches for the synthesis of these compounds are of interest. Recently, we reported a one-step synthesis of tetraarylstannanes with the general structure Ar_4Sn using the reaction of aryl iodides with copper bronze (Shaikh *et al.*, 2006). Here, we describe the crystal structure of the title compound, (I), which was synthesized during our efforts to optimize this novel synthetic approach further (Fig. 1).



(I)

The title compound crystallizes in monoclinic space group $P2_1/n$. This is in contrast with numerous other tetraarylstannanes, which crystallize in tetragonal space groups (Belsky *et al.*, 1983; Karipides *et al.*, 1974; Karipides & Oertel, 1977; Karipides & Wolfe, 1975; Smith *et al.*, 1994; Wharf *et al.*, 1990; Wharf & Bélanger-Gariépy, 2003; Wharf & Lebuis, 2000; Wharf & Simard, 1987; Young *et al.*, 2005; Chieh & Trotter, 1970; Shaikh *et al.*, 2006), and their molecules in many cases occupy special positions with crystallographic symmetry $\overline{4}$. In some papers (Wharf & Simard, 1995), it is implied that the ability to occupy high-symmetry special positions leads to a dense packing of these compounds in the solid state. There are, however, several papers that report crystal structures of tetraarylstannanes in non-tetragonal space groups, such as *Pbca*, $P\overline{1}$, $P2_1/c$ or $C2/c$ (Shaikh *et al.*, 2006; Shaikh *et al.*, 2007; Wharf & Simard, 1991; Wharf & Simard, 1995; Wharf & Lebuis, 2003; Ara *et al.*, 2004; Ross *et al.*, 1994; Ng, 1997). Many of the compounds belonging to this group have relatively large

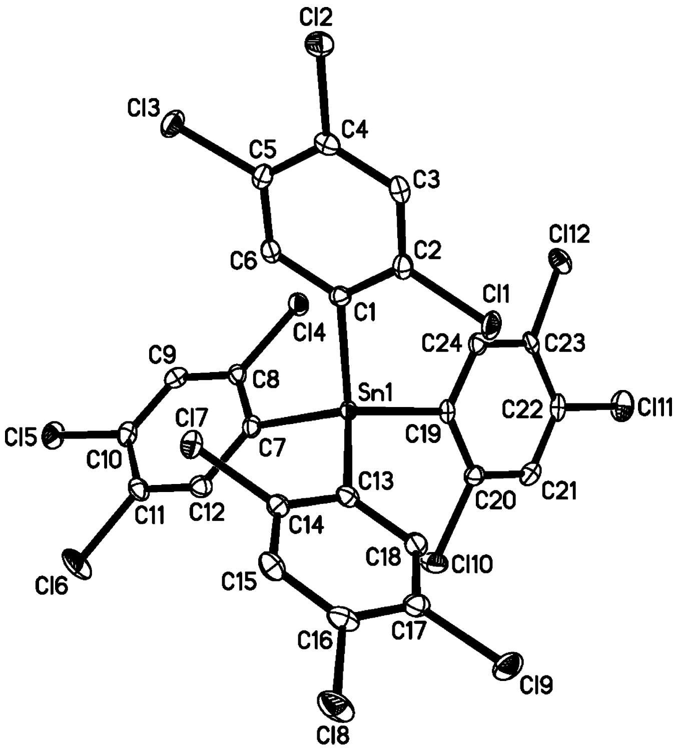


Figure 1
The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted.

substituents, which would have caused loss of close packing in the tetragonal space groups as a result of the steric requirements of the substituents.

Even though the molecule of the title compound occupies a general position in the crystal structure, it has approximate molecular geometry $\overline{4}$ in the solid state, and has a single principal symmetry axis running through the mid-points of C1···C13 and C7···C19. The most significant deviation from $\overline{4}$ molecular symmetry becomes apparent when analyzing the angles β and θ, which are defined with respect to the symmetry axis (Wharf & Simard, 1995; Hutchings *et al.*, 1975). Four β angles are expected to have equal values for ideal $\overline{4}$ geometry; two θ angles should also be equal. One can see, however, that the molecule of the title compound shows significant variation in the β angles [C1—Sn1—C19 = 108.96 (10)°, C7—Sn1—C13 = 110.47 (10)°, C7—Sn1—C1 = 109.47 (10)° and C13—Sn1—C19 = 115.94 (10)°] as well as a noticeable difference between the θ angles [C1—Sn1—C13 = 103.90 (10)° and C7—Sn1—C19 = 107.94 (10)°].

Experimental

The title compound was synthesized in one step using the reaction of 2,4,5-trichloro-1-iodobenzene with copper bronze at 503 K (Shaikh *et al.*, 2006). Crystals suitable for the X-ray diffraction study were obtained by slow evaporation of the solvent from a solution of (I) in chloroform.

Crystal data

$[Sn(C_6H_2Cl_3)_4]$
$M_r = 840.39$
Monoclinic, $P2_1/n$
$a = 7.9536$ (4) Å
$b = 33.8974$ (15) Å
$c = 11.2442$ (5) Å
$\beta = 109.584$ (2)°
$V = 2856.1$ (2) Å^3
$Z = 4$
Cu $K\alpha$ radiation
$\mu = 17.60$ mm^{-1}
$T = 90.0$ (2) K
0.08 × 0.08 × 0.04 mm

Data collection

Bruker X8 Proteum diffractometer
Absorption correction: multi-scan (*SADABS* in *APEX2*; Bruker, 2004)
$T_{min} = 0.328$, $T_{max} = 0.543$
27165 measured reflections
5021 independent reflections
4856 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.059$
$S = 1.09$
5021 reflections
335 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.65$ e Å^{-3}
$\Delta\rho_{min} = -0.55$ e Å^{-3}

The H atoms were placed in idealized positions (C—H = 0.95 Å) and included in the subsequent refinement in the riding-model approximation with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1994); software used to prepare material for publication: *SHELX97*-2 (Sheldrick, 1997) and local procedures.

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