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Key indicators

Single-crystal X-ray study
 $T = 90$ K
Mean $\sigma(C-C) = 0.004$ Å
 R factor = 0.024
 wR factor = 0.059
Data-to-parameter ratio = 15.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

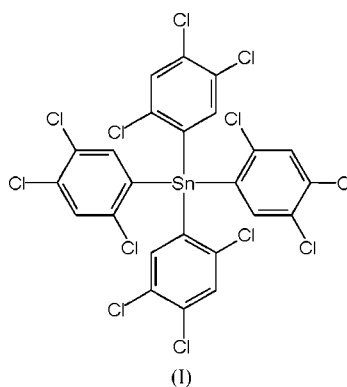
Tetrakis(2,4,5-trichlorophenyl)stannane

The molecule of the title compound, $[\text{Sn}(\text{C}_6\text{H}_2\text{Cl}_3)_4]$, occupies
a general position in the crystal structure, but shows an
approximate $\bar{4}$ molecular symmetry.

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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).The title compound crystallizes in monoclinic space group
 $P2_1/n$. This is in contrast with numerous other tetraaryl-
stannanes, 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 & Lehuis, 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 $\bar{4}$. 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
 $Pbca$, $P\bar{1}$, $P2_1/c$ or $C2/c$ (Shaikh *et al.*, 2006; Shaikh *et al.*, 2007;
Wharf & Simard, 1991; Wharf & Simard, 1995; Wharf &
Lehuis, 2003; Ara *et al.*, 2004; Ross *et al.*, 1994; Ng, 1997). Many
of the compounds belonging to this group have relatively large

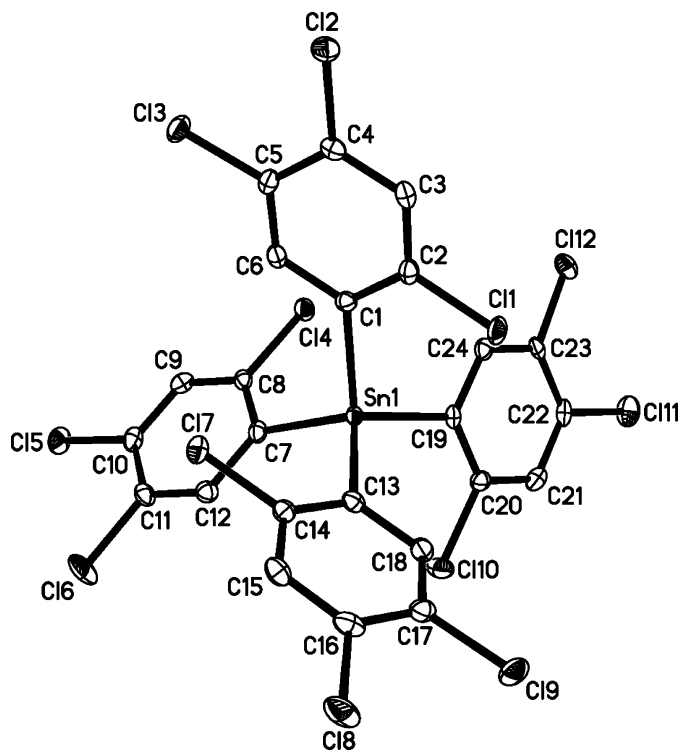


Figure 1

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 $\bar{4}$ 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 $\bar{4}$ 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 $\bar{4}$ 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(C₆H₂Cl₃)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) Å³
 $Z = 4$
 Cu K α radiation
 $\mu = 17.60$ mm⁻¹
 $T = 90.0$ (2) K
 $0.08 \times 0.08 \times 0.04$ 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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.040$

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
 $\Delta\rho_{\text{max}} = 0.65$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.55$ 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 $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

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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