

## Tetrakis(4-fluorophenyl)stannane

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## Key indicators

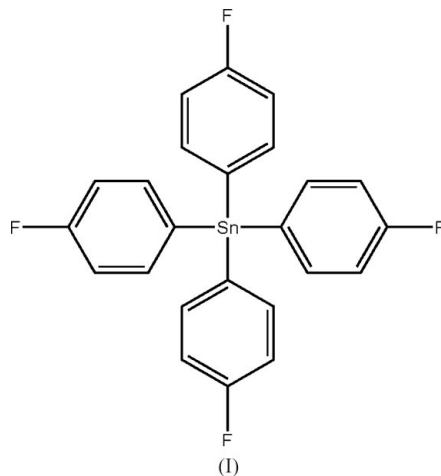
Single-crystal X-ray study  
 $T = 90$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.023  
 $wR$  factor = 0.061  
Data-to-parameter ratio = 13.6For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.The title compound,  $[\text{Sn}(\text{C}_6\text{H}_4\text{F})_4]$ , displays significant deviation from ideal tetrahedral molecular symmetry.

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## Comment

Organotin(IV) compounds are used for a wide range of applications such as PVC stabilizers, oxidizing agents for rubber, catalysts for polymer synthesis and agricultural fungicides (Veith *et al.*, 2004). They are also under investigation for various biomedical applications due to their stability in air and towards water (Pellerito *et al.*, 2006; Gielen, 2002; Veith *et al.*, 2004). Symmetrical aryl-substituted organotin(IV) compounds can be synthesized, for example, by reaction of a Grignard reagent or an organolithium compound with  $\text{SnCl}_4$  (Davies, 2004). We have recently described how a variety of substituted tetraarylstannanes can be synthesized *via* a copper-bronze-mediated coupling reaction (Shaikh *et al.*, 2006). We report here the crystal structure of the title compound, (I), which was synthesized from 1-fluoro-4-iodobenzene using this novel reaction with copper bronze.



Many functionalized tetraarylstannane derivatives, especially with small *para* substituents, crystallize in tetragonal space groups and have tetrahedral symmetry (Belsky *et al.*, 1983; Karipides *et al.*, 1974; Karipides & Oertel, 1977; Karipides & Wolfe, 1975; Smith *et al.*, 1994; Wharf & Bélanger-Gariépy, 2003; Wharf & Lebus, 2000; Wharf & Simard, 1987; Wharf *et al.*, 1990; Young *et al.*, 2005). Although the 4-fluoro group is comparatively small, the title compound does not follow this trend and crystallizes in the monoclinic space group  $P2_1/c$ . The title compound has a principal symmetry axis through the mid-point of C1–C13 and C7–C19 *via* the Sn1 atom, but does not display ideal tetrahedral symmetry.

The angles  $\beta$  and  $\theta$ , which are defined by this symmetry axis (Hutchings *et al.*, 1975; Wharf & Simard, 1995), indicate a significant deviation from tetrahedral symmetry. Specifically, there are four angles  $\beta$  [106.97 (9) (C1–Sn1–C19), 111.36 (9) (C1–Sn1–C7), 111.75 (10) (C7–Sn1–C13) and 107.06 (10)° (C13–Sn1–C19)] and two angles  $\theta$  [111.49 (9) (C1–Sn1–C13) and 109.01 (10)° (C7–Sn1–C19)]. The dihedral angles  $\varphi$ , which describe the aryl-ring orientations with respect to the C–Sn–C plane that contains the principal axis are 52.2 (8) (ring C1–C6), 51.4 (9) (ring C7–12), –131.1 (9) (ring C13–C18) and 72.6 (9)° (ring C19–C24).

### Experimental

The title compound, (I), was synthesized in one step using the reaction of copper bronze with 1-fluoro-4-iodobenzene at 503 K (Shaikh *et al.*, 2006). Crystal of (I) were obtained by slow crystallization of a hexane–ethyl (1:1 *v/v*) acetate solution.

#### Crystal data

[Sn(C <sub>6</sub> H <sub>4</sub> F) <sub>4</sub> ]	$V = 1989.6 (7) \text{ \AA}^3$
$M_r = 499.06$	$Z = 4$
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation
$a = 9.4775 (19) \text{ \AA}$	$\mu = 10.61 \text{ mm}^{-1}$
$b = 19.873 (4) \text{ \AA}$	$T = 90.0 (2) \text{ K}$
$c = 11.029 (2) \text{ \AA}$	$0.20 \times 0.06 \times 0.04 \text{ mm}$
$\beta = 106.69 (3)^\circ$	

#### Data collection

Bruker X8 Proteum diffractometer	40140 measured reflections
Absorption correction: multi-scan (SADABS in APEX2; Bruker, 2004)	3582 independent reflections
$T_{\min} = 0.511$ , $T_{\max} = 0.652$	3457 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.040$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.023$	263 parameters
$wR(F^2) = 0.061$	H-atom parameters constrained
$S = 1.14$	$\Delta\rho_{\text{max}} = 0.48 \text{ e \AA}^{-3}$
3582 reflections	$\Delta\rho_{\text{min}} = -0.45 \text{ e \AA}^{-3}$

H atoms were placed in idealized positions (C–H = 0.95 Å) and refined as riding, 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: XP in SHELXTL (Sheldrick, 1994); software used to prepare material for publication: SHELX97-2 (Sheldrick, 1997) and local procedures.

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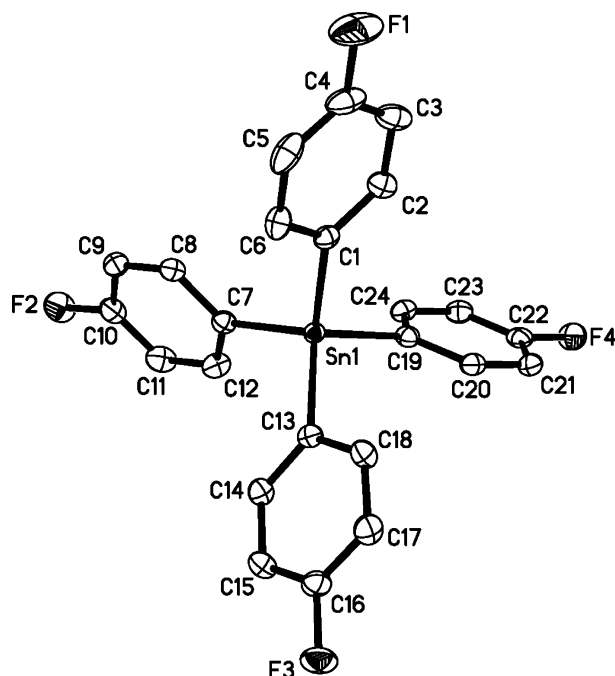


Figure 1

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.

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