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Tetrakis(4-methyl-2-thienyl)tin(IV)

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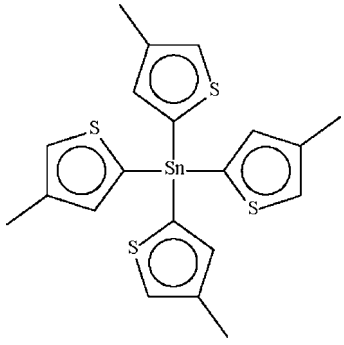
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.012; wR factor = 0.028; data-to-parameter ratio = 19.8.

The molecule of the title compound, $[Sn(C_5H_5S)_4]$, lies on a special position of $\overline{4}$ site symmetry. The Sn^{IV} atom shows a slightly distorted tetrahedral coordination.

Related literature

For the structure of tetrakis(2-thienyl)tin, see: Karipides *et al.* (1977). For the synthesis, see: Kumar Das *et al.* (1987).



Experimental

Crystal data

$[Sn(C_5H_5S)_4]$
M_r = 507.29
Tetragonal, $I\overline{4}$
a = 11.6286 (9) Å
c = 7.5918 (6) Å
V = 1026.6 (1) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.65 mm^{-1}
T = 100 (2) K
0.30 × 0.25 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.637, T_{max} = 0.852
2948 measured reflections
1151 independent reflections
1149 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.012
$wR(F^2)$ = 0.028
S = 1.01
1151 reflections
58 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Absolute structure: Flack (1983), 513 Friedel pairs
Flack parameter: 0.005 (14)

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2670).

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supporting information

Acta Cryst. (2008). E**64**, m1410 [doi:10.1107/S1600536808032790]

Tetrakis(4-methyl-2-thienyl)tin(IV)

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S1. Experimental

The title compound was synthesized as reported previously (Kumar Das *et al.*, 1987). Single crystals were obtained upon recrystallization from chloroform.

S2. Refinement

H-atoms were placed in calculated positions (C-H = 0.95-0.98 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2–1.5U_{eq}(C).

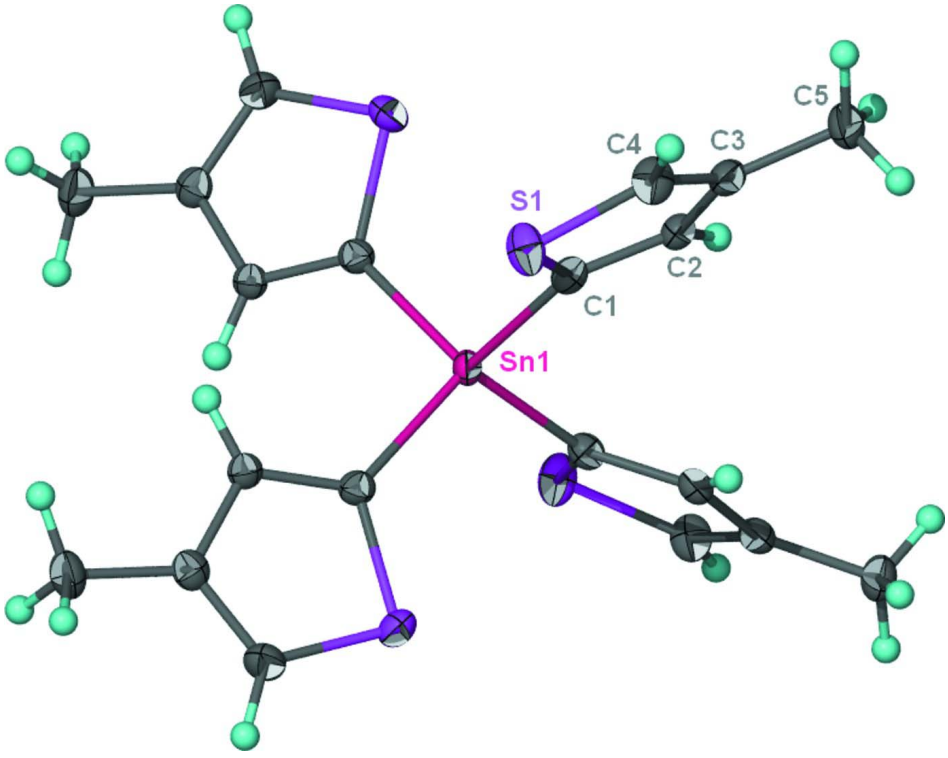

Figure 1

Displacement ellipsoid plot (Barbour, 2001) of $[Sn(C_5H_5S)_4]$ at the 70% probability level. H atoms are drawn as spheres of arbitrary radii.

Tetrakis(4-methyl-2-thienyl)tin(IV)

Crystal data

$[Sn(C_5H_5S)_4]$
$M_r = 507.29$
Tetragonal, $I\bar{4}$
Hall symbol: I -4
$a = 11.6286$ (9) Å
$c = 7.5918$ (6) Å
$V = 1026.6$ (1) Å^3
$Z = 2$
$F(000) = 508$
$D_x = 1.641$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2958 reflections
$\theta = 2.5$–$28.3°$
$\mu = 1.65$ mm^{-1}
$T = 100$ K
Prism, colourless
0.30 × 0.25 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.637$, $T_{max} = 0.852$
2948 measured reflections
1151 independent reflections
1149 reflections with $I > 2\sigma(I)$
$R_{int} = 0.014$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.5°$
$h = -15 \rightarrow 14$
$k = -15 \rightarrow 13$
$l = -9 \rightarrow 8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.012$
$wR(F^2) = 0.028$
$S = 1.01$
1151 reflections
58 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0145P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}
Absolute structure: Flack (1983), 513 Friedel pairs
Absolute structure parameter: 0.005 (14)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.5000	0.5000	0.5000	0.01202 (5)
S1	0.36597 (3)	0.74692 (3)	0.61422 (5)	0.02012 (9)
C1	0.46144 (12)	0.63979 (12)	0.6694 (2)	0.0140 (3)
C2	0.50206 (12)	0.65832 (13)	0.8364 (2)	0.0134 (3)
H2	0.5562	0.6088	0.8914	0.016*
C3	0.45677 (14)	0.75770 (14)	0.9212 (2)	0.0154 (3)
C4	0.38176 (14)	0.81447 (13)	0.8139 (2)	0.0192 (3)
H4	0.3429	0.8832	0.8459	0.023*
C5	0.48542 (16)	0.79485 (16)	1.1056 (2)	0.0206 (4)
H5A	0.4919	0.8788	1.1097	0.031*
H5B	0.5586	0.7602	1.1414	0.031*
H5C	0.4244	0.7697	1.1859	0.031*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01360 (6)	0.01360 (6)	0.00885 (9)	0.000	0.000	0.000
S1	0.0221 (2)	0.0223 (2)	0.0160 (2)	0.00775 (16)	−0.00468 (16)	0.00016 (16)
C1	0.0138 (7)	0.0138 (7)	0.0144 (8)	0.0010 (5)	0.0011 (6)	0.0019 (6)
C2	0.0133 (6)	0.0140 (7)	0.0129 (8)	0.0000 (5)	0.0011 (6)	0.0020 (6)
C3	0.0165 (8)	0.0151 (8)	0.0146 (8)	−0.0017 (6)	0.0023 (6)	0.0011 (6)
C4	0.0220 (8)	0.0172 (8)	0.0185 (9)	0.0055 (6)	0.0014 (7)	−0.0008 (7)
C5	0.0267 (9)	0.0213 (9)	0.0139 (9)	−0.0005 (7)	0.0007 (7)	−0.0030 (7)

Geometric parameters (Å, º)

Sn1—C1^{i}	2.1209 (15)	C2—H2	0.95
Sn1—C1	2.1209 (15)	C3—C4	1.364 (2)
Sn1—C1^{ii}	2.1209 (15)	C3—C5	1.502 (2)
Sn1—C1^{iii}	2.1209 (15)	C4—H4	0.95
S1—C4	1.7173 (16)	C5—H5A	0.98
S1—C1	1.7206 (15)	C5—H5B	0.98
C1—C2	1.370 (2)	C5—H5C	0.98
C2—C3	1.424 (2)		
C1^{i}—Sn1—C1	111.58 (4)	C4—C3—C2	111.07 (15)
C1^{i}—Sn1—C1^{ii}	105.32 (8)	C4—C3—C5	124.00 (16)
C1—Sn1—C1^{ii}	111.58 (4)	C2—C3—C5	124.92 (16)
C1^{i}—Sn1—C1^{iii}	111.58 (4)	C3—C4—S1	111.98 (12)
C1—Sn1—C1^{iii}	105.32 (8)	C3—C4—H4	124.0
C1^{ii}—Sn1—C1^{iii}	111.58 (4)	S1—C4—H4	124.0
C4—S1—C1	92.70 (8)	C3—C5—H5A	109.5
C2—C1—S1	109.51 (12)	C3—C5—H5B	109.5
C2—C1—Sn1	127.51 (11)	H5A—C5—H5B	109.5
S1—C1—Sn1	122.93 (8)	C3—C5—H5C	109.5
C1—C2—C3	114.74 (14)	H5A—C5—H5C	109.5
C1—C2—H2	122.6	H5B—C5—H5C	109.5
C3—C2—H2	122.6		
C4—S1—C1—C2	0.03 (12)	S1—C1—C2—C3	0.28 (17)
C4—S1—C1—Sn1	177.81 (9)	Sn1—C1—C2—C3	−177.37 (11)
C1^{i}—Sn1—C1—C2	149.39 (12)	C1—C2—C3—C4	−0.54 (19)
C1^{ii}—Sn1—C1—C2	−93.09 (10)	C1—C2—C3—C5	178.39 (14)
C1^{iii}—Sn1—C1—C2	28.15 (11)	C2—C3—C4—S1	0.54 (17)
C1^{i}—Sn1—C1—S1	−27.98 (10)	C5—C3—C4—S1	−178.40 (12)
C1^{ii}—Sn1—C1—S1	89.54 (12)	C1—S1—C4—C3	−0.34 (13)
C1^{iii}—Sn1—C1—S1	−149.22 (11)		

Symmetry codes: (i) −*y*+1, *x*, −*z*+1; (ii) *y*, −*x*+1, −*z*+1; (iii) −*x*+1, −*y*+1, *z*.