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

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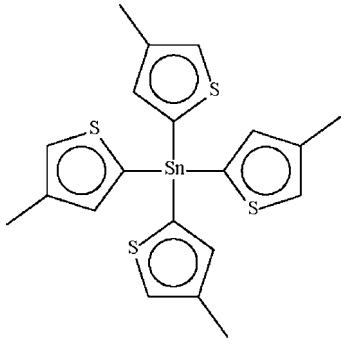
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.012; wR factor = 0.028; data-to-parameter ratio = 19.8.

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).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Karipides, A., Reed, A. T., Haller, D. A. & Hayes, F. (1977). *Acta Cryst.* B**33**, 950–951.
Kumar Das, V. G., Lo, K. M. & Blunden, S. J. (1987). *J. Organomet. Chem.* **334**, 307–322.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2008). *publCIF*. In preparation.

supplementary materials

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

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

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Experimental

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

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).

Figures

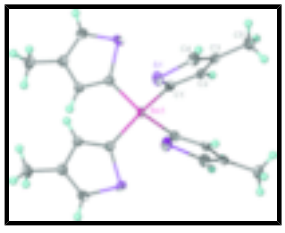

Fig. 1. Displacement ellipsoid plot (Barbour, 2001) of $[Sn(C_5H_5S)_4]$ at the 70% probability level. H atoms are drawn as spheres of arbitrary radii.

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

Crystal data

$[Sn(C_5H_5S)_4]$	$Z = 2$
$M_r = 507.29$	$F_{000} = 508$
Tetragonal, $I\bar{4}$	$D_x = 1.641$ Mg m^{-3}
Hall symbol: I -4	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 11.6286$ (9) Å	Cell parameters from 2958 reflections
$b = 11.6286$ Å	$\theta = 2.5$–28.3º
$c = 7.5918$ (6) Å	$\mu = 1.65$ mm^{-1}
$\alpha = 90$º	$T = 100$ (2) K
$\beta = 90$º	Prism, colourless
$\gamma = 90$º	0.30 × 0.25 × 0.10 mm
$V = 1026.6$ (1) Å^3	

Data collection

Bruker SMART APEX diffractometer	1151 independent reflections

Radiation source: fine-focus sealed tube	1149 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.014$
$T = 100(2)$ K	$\theta_{max} = 27.5^{o}$
ω scans	$\theta_{min} = 2.5^{o}$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -15\rightarrow14$
$T_{min} = 0.637$, $T_{max} = 0.852$	$k = -15\rightarrow13$
2948 measured reflections	$l = -9\rightarrow8$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.012$	$w = 1/[\sigma^2(F_o^2) + (0.0145P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.028$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.01$	$\Delta\rho_{max} = 0.45$ e Å^{-3}
1151 reflections	$\Delta\rho_{min} = -0.21$ e Å^{-3}
58 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 513 Friedel pairs
Secondary atom site location: difference Fourier map	Flack 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 (Å^2)

	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, °)

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*.

Fig. 1