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catena-Poly[[triphenyltin(IV)]-μ-3-methylphenylseleninato-κ^2O:O']

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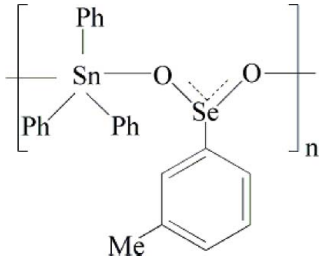
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.009 Å; R factor = 0.038; wR factor = 0.097; data-to-parameter ratio = 14.5.

In the polymeric title coordination compound, $[Sn(C_6H_5)_3(C_7H_7O_2Se)]_n$, the Sn^{IV} atom has a distorted trigonal–bipyramidal geometry, with two O atoms from two symmetry-related bridging seleninate ligands in axial positions and three phenyl groups in the equatorial plane. In the crystal, the complex exhibits a zigzag chain structure running parallel to the c axis. An intrachain C—H···O hydrogen bond is observed.

Related literature

For the biological activity of organotin compounds, see: Dubey & Roy (2003). For related structures, see: Chandrasekhar *et al.* (1992); Guo *et al.* (2011).



Experimental

Crystal data

$[Sn(C_6H_5)_3(C_7H_7O_2Se)]$
M_r = 552.08
Monoclinic, $P2_1/c$
a = 12.3293 (11) Å
b = 14.3519 (16) Å
c = 12.2865 (13) Å
β = 94.324 (1)°
V = 2167.9 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.88 mm^{-1}
T = 298 K
0.35 × 0.14 × 0.10 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.433, T_{max} = 0.762
10632 measured reflections
3821 independent reflections
2802 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.097
S = 1.09
3821 reflections
263 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9···O1	0.93	2.57	3.487 (7)	169

Data collection: *SMART* (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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2663).

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supplementary materials

Acta Cryst. (2011). E**67**, m1809 [**doi:10.1107/S1600536811049245**]

catena-Poly[[triphenyltin(IV)]-μ-3-methylphenylseleninato-κ^2O:O']

J. Ru and R. Zhang

Comment

Organotin compounds have been attracting more and more attention due to their wide range of industrial applications and biological activities (Dubey & Roy, 2003). As a part of our ongoing investigations in this field (Guo *et al.*, 2011), we have synthesized the title compound and present its crystal structure herein.

The asymmetric unit of the title compound is shown in Fig. 1. An extended one-dimensional zigzag chain structure running parallel to the *c* axis is formed by the bridging role of the 3-methylphenylseleninate anions (Fig. 2). The Se—O bond distances in the compound (Se1—O1 = 1.674 (4) Å; Se1—O2 = 1.698 (3) Å) are comparable to those found in a related polymeric organotin complex (Chandrasekhar *et al.*, 1992). The Sn atom is five-coordinate in a slightly distorted trigonal-bipyramidal coordination geometry, provided by the phenyl groups in the equatorial positions and two O atoms of symmetry related 3-methylphenylseleninate groups in the axial positions. An intrachain C—H···O hydrogen bond is observed (Table 1).

Experimental

The reaction was carried out under a nitrogen atmosphere. 3-Tolueneseleninic acid (1 mmol) and sodium ethoxide (1 mmol) were added to a stirred solution of methanol (30 ml) in a Schlenk flask and stirred for 30 min. Triphenyltin chloride (1 mmol) was then added to the reactor and the reaction mixture was stirred for 10 h at room temperature. The resulting clear solution was evaporated under vacuum. The product was crystallized from a solution of ether to yield colourless blocks of the title compound (yield 60%). Anal. Calcd (%) for $C_{25}H_{22}O_2Sn_1Se_1$ (Mr = 552.08): C,54.39; H, 4.02. Found (%): C, 54.25; H, 4.28.

Refinement

The H atoms were positioned geometrically, with methyl C—H distances of 0.96 Å and aromatic C—H distances of 0.93 Å, and refined as riding on their parent atoms, with U_{iso}(H) = 1.5U_{eq}(C) for the methyl group or U_{iso}(H) = 1.2U_{eq}(C) for the phenyl groups.

Figures

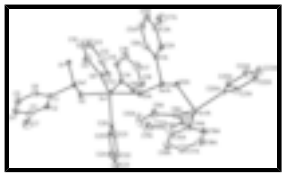

Fig. 1. The asymmetric unit of the title compound, showing 50% probability displacement ellipsoids. H atoms have been omitted for clarity.

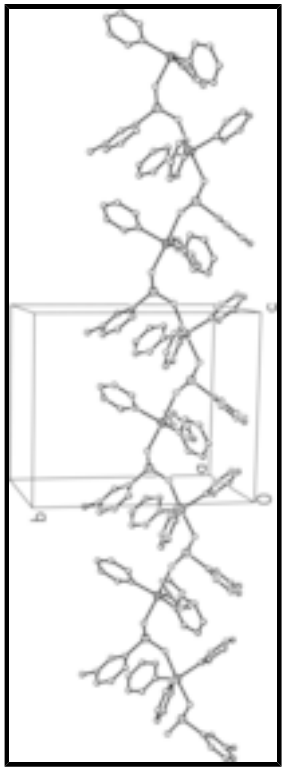

Fig. 2. View of the one-dimensional zigzag chain structure running parallel to the *c* axis in the title compound. H atoms have been omitted for clarity.

catena-Poly[[triphenyltin(IV)]-μ-3-methylphenylseleninato- $\kappa^2O:O'$]

Crystal data

$[Sn(C_6H_5)_3(C_7H_7O_2Se)]$	$F(000) = 1088$
$M_r = 552.08$	$D_x = 1.691$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 3292 reflections
$a = 12.3293$ (11) Å	$\theta = 2.7$–$27.0°$
$b = 14.3519$ (16) Å	$\mu = 2.88$ mm^{-1}
$c = 12.2865$ (13) Å	$T = 298$ K
$\beta = 94.324$ (1)°	Block, colourless
$V = 2167.9$ (4) Å^3	0.35 × 0.14 × 0.10 mm
$Z = 4$	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	3821 independent reflections
Radiation source: fine-focus sealed tube	2802 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.061$
phi and ω scans	$\theta_{max} = 25.0°$, $\theta_{min} = 2.7°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)	$h = -14 \rightarrow 14$
$T_{min} = 0.433$, $T_{max} = 0.762$	$k = -17 \rightarrow 17$

10632 measured reflections	$l = -14 \rightarrow 12$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.038$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.097$	H-atom parameters constrained
$S = 1.09$	$w = 1/[\sigma^2(F_o^2) + (0.0361P)^2 + 1.7781P]$ where $P = (F_o^2 + 2F_c^2)/3$
3821 reflections	$(\Delta/\sigma)_{max} = 0.001$
263 parameters	$\Delta\rho_{max} = 1.11$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.71$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.70340 (3)	0.19810 (3)	0.84922 (3)	0.02761 (13)
Se1	0.77442 (5)	0.15274 (4)	0.58249 (4)	0.03037 (17)
O1	0.7026 (3)	0.2382 (3)	0.5185 (3)	0.0369 (10)
O2	0.7000 (3)	0.1284 (3)	0.6898 (3)	0.0358 (10)
C1	0.7357 (5)	0.0477 (4)	0.4897 (4)	0.0301 (13)
C2	0.8174 (5)	−0.0095 (4)	0.4585 (5)	0.0391 (15)
H2	0.8887	0.0016	0.4855	0.047*
C3	0.7952 (6)	−0.0832 (5)	0.3876 (5)	0.0516 (18)
C4	0.6892 (6)	−0.0984 (5)	0.3507 (5)	0.0537 (19)
H4	0.6725	−0.1482	0.3041	0.064*
C5	0.6067 (6)	−0.0415 (5)	0.3812 (5)	0.0542 (18)
H5	0.5354	−0.0530	0.3545	0.065*
C6	0.6288 (5)	0.0312 (4)	0.4498 (5)	0.0382 (15)
H6	0.5731	0.0697	0.4699	0.046*
C7	0.8869 (7)	−0.1441 (6)	0.3487 (7)	0.089 (3)
H7A	0.8624	−0.2075	0.3418	0.133*
H7B	0.9488	−0.1409	0.4008	0.133*

H7C	0.9068	−0.1220	0.2792	0.133*
C8	0.5467 (4)	0.2559 (4)	0.8132 (4)	0.0289 (12)
C9	0.5205 (5)	0.2946 (5)	0.7122 (5)	0.0475 (17)
H9	0.5676	0.2878	0.6570	0.057*
C10	0.4236 (6)	0.3440 (6)	0.6922 (6)	0.066 (2)
H10	0.4070	0.3706	0.6239	0.080*
C11	0.3525 (6)	0.3539 (5)	0.7720 (7)	0.061 (2)
H11	0.2886	0.3878	0.7586	0.073*
C12	0.3767 (5)	0.3133 (5)	0.8715 (6)	0.0499 (18)
H12	0.3278	0.3180	0.9253	0.060*
C13	0.4728 (5)	0.2655 (4)	0.8929 (5)	0.0394 (15)
H13	0.4887	0.2392	0.9614	0.047*
C14	0.8439 (5)	0.2784 (4)	0.8187 (4)	0.0299 (13)
C15	0.8425 (5)	0.3467 (4)	0.7412 (5)	0.0439 (16)
H15	0.7786	0.3574	0.6977	0.053*
C16	0.9327 (6)	0.4001 (5)	0.7254 (6)	0.0566 (19)
H16	0.9288	0.4471	0.6731	0.068*
C17	1.0270 (6)	0.3841 (5)	0.7861 (6)	0.058 (2)
H17	1.0883	0.4196	0.7750	0.070*
C18	1.0322 (5)	0.3148 (5)	0.8646 (6)	0.0540 (19)
H18	1.0969	0.3039	0.9066	0.065*
C19	0.9419 (5)	0.2624 (4)	0.8804 (5)	0.0394 (15)
H19	0.9460	0.2155	0.9329	0.047*
C20	0.7300 (5)	0.0694 (4)	0.9337 (4)	0.0312 (13)
C21	0.6583 (5)	0.0405 (4)	1.0097 (5)	0.0430 (16)
H21	0.5969	0.0757	1.0214	0.052*
C22	0.6796 (7)	−0.0412 (5)	1.0677 (5)	0.057 (2)
H22	0.6319	−0.0607	1.1182	0.069*
C23	0.7689 (8)	−0.0929 (5)	1.0516 (6)	0.066 (2)
H23	0.7818	−0.1477	1.0908	0.079*
C24	0.8394 (7)	−0.0651 (5)	0.9787 (7)	0.065 (2)
H24	0.9013	−0.1003	0.9690	0.077*
C25	0.8198 (5)	0.0154 (4)	0.9186 (5)	0.0472 (17)
H25	0.8678	0.0332	0.8675	0.057*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0338 (2)	0.0285 (2)	0.0204 (2)	0.00111 (18)	0.00173 (15)	0.00267 (18)
Se1	0.0344 (3)	0.0338 (3)	0.0231 (3)	0.0015 (3)	0.0036 (2)	−0.0007 (3)
O1	0.053 (3)	0.039 (2)	0.018 (2)	0.009 (2)	0.0011 (18)	−0.0015 (18)
O2	0.053 (3)	0.038 (2)	0.016 (2)	−0.007 (2)	0.0051 (17)	−0.0003 (18)
C1	0.050 (4)	0.026 (3)	0.015 (3)	0.003 (3)	0.007 (2)	0.000 (2)
C2	0.045 (4)	0.041 (3)	0.032 (3)	0.010 (3)	0.004 (3)	0.002 (3)
C3	0.077 (5)	0.047 (4)	0.032 (4)	0.021 (4)	0.014 (4)	−0.004 (3)
C4	0.086 (6)	0.043 (4)	0.033 (4)	−0.009 (4)	0.005 (4)	−0.004 (3)
C5	0.059 (5)	0.059 (4)	0.045 (4)	−0.003 (4)	0.000 (3)	0.000 (4)
C6	0.038 (4)	0.035 (3)	0.042 (4)	−0.001 (3)	0.005 (3)	−0.002 (3)

C7	0.106 (7)	0.092 (7)	0.070 (6)	0.040 (6)	0.017 (5)	−0.030 (5)
C8	0.034 (3)	0.023 (3)	0.029 (3)	0.001 (3)	0.000 (2)	−0.001 (3)
C9	0.047 (4)	0.065 (4)	0.032 (4)	0.012 (3)	0.009 (3)	0.010 (3)
C10	0.058 (5)	0.091 (6)	0.050 (5)	0.022 (4)	0.003 (4)	0.030 (4)
C11	0.042 (4)	0.070 (5)	0.070 (5)	0.022 (4)	0.003 (4)	0.003 (4)
C12	0.036 (4)	0.066 (5)	0.050 (4)	−0.001 (3)	0.014 (3)	−0.015 (4)
C13	0.038 (4)	0.050 (4)	0.031 (3)	−0.002 (3)	0.008 (3)	0.001 (3)
C14	0.037 (3)	0.030 (3)	0.024 (3)	0.001 (2)	0.009 (2)	−0.004 (3)
C15	0.051 (4)	0.049 (4)	0.031 (4)	0.000 (3)	−0.005 (3)	0.008 (3)
C16	0.064 (5)	0.057 (4)	0.051 (5)	−0.011 (4)	0.017 (4)	0.012 (4)
C17	0.048 (4)	0.067 (5)	0.063 (5)	−0.018 (4)	0.018 (4)	0.005 (4)
C18	0.030 (4)	0.066 (5)	0.065 (5)	0.001 (3)	−0.003 (3)	−0.009 (4)
C19	0.038 (4)	0.039 (3)	0.041 (4)	0.006 (3)	0.002 (3)	0.003 (3)
C20	0.046 (4)	0.028 (3)	0.018 (3)	−0.003 (3)	−0.003 (2)	0.000 (2)
C21	0.056 (4)	0.039 (4)	0.034 (4)	−0.009 (3)	0.007 (3)	0.000 (3)
C22	0.089 (6)	0.053 (4)	0.030 (4)	−0.025 (4)	0.001 (4)	0.011 (3)
C23	0.103 (7)	0.040 (4)	0.051 (5)	−0.002 (4)	−0.015 (5)	0.018 (4)
C24	0.081 (6)	0.042 (4)	0.069 (5)	0.022 (4)	−0.008 (4)	−0.005 (4)
C25	0.056 (4)	0.040 (4)	0.046 (4)	0.010 (3)	0.002 (3)	0.003 (3)

Geometric parameters (Å, °)

Sn1—C8	2.119 (5)	C10—H10	0.9300
Sn1—C20	2.132 (5)	C11—C12	1.367 (10)
Sn1—C14	2.136 (5)	C11—H11	0.9300
Sn1—O2	2.197 (4)	C12—C13	1.378 (9)
Sn1—O1^{i}	2.273 (4)	C12—H12	0.9300
Se1—O1	1.674 (4)	C13—H13	0.9300
Se1—O2	1.698 (3)	C14—C15	1.367 (8)
Se1—C1	1.928 (5)	C14—C19	1.397 (8)
O1—Sn1^{ii}	2.273 (4)	C15—C16	1.376 (9)
C1—C2	1.376 (7)	C15—H15	0.9300
C1—C6	1.391 (8)	C16—C17	1.354 (10)
C2—C3	1.384 (9)	C16—H16	0.9300
C2—H2	0.9300	C17—C18	1.383 (10)
C3—C4	1.368 (10)	C17—H17	0.9300
C3—C7	1.533 (9)	C18—C19	1.369 (9)
C4—C5	1.378 (9)	C18—H18	0.9300
C4—H4	0.9300	C19—H19	0.9300
C5—C6	1.356 (9)	C20—C25	1.376 (8)
C5—H5	0.9300	C20—C21	1.396 (8)
C6—H6	0.9300	C21—C22	1.386 (9)
C7—H7A	0.9600	C21—H21	0.9300
C7—H7B	0.9600	C22—C23	1.354 (10)
C7—H7C	0.9600	C22—H22	0.9300
C8—C9	1.376 (8)	C23—C24	1.356 (10)
C8—C13	1.393 (8)	C23—H23	0.9300
C9—C10	1.395 (9)	C24—C25	1.382 (9)
C9—H9	0.9300	C24—H24	0.9300

C10—C11	1.371 (10)	C25—H25	0.9300
C8—Sn1—C20	123.1 (2)	C9—C10—H10	119.6
C8—Sn1—C14	119.4 (2)	C12—C11—C10	119.2 (6)
C20—Sn1—C14	117.1 (2)	C12—C11—H11	120.4
C8—Sn1—O2	92.10 (18)	C10—C11—H11	120.4
C20—Sn1—O2	91.81 (17)	C11—C12—C13	120.6 (6)
C14—Sn1—O2	92.88 (17)	C11—C12—H12	119.7
C8—Sn1—O1^{i}	88.08 (18)	C13—C12—H12	119.7
C20—Sn1—O1^{i}	85.07 (17)	C12—C13—C8	120.9 (6)
C14—Sn1—O1^{i}	90.18 (17)	C12—C13—H13	119.5
O2—Sn1—O1^{i}	176.38 (13)	C8—C13—H13	119.5
O1—Se1—O2	102.58 (19)	C15—C14—C19	117.5 (5)
O1—Se1—C1	101.3 (2)	C15—C14—Sn1	122.8 (4)
O2—Se1—C1	100.0 (2)	C19—C14—Sn1	119.8 (4)
Se1—O1—Sn1^{ii}	133.3 (2)	C14—C15—C16	122.0 (6)
Se1—O2—Sn1	128.6 (2)	C14—C15—H15	119.0
C2—C1—C6	119.6 (5)	C16—C15—H15	119.0
C2—C1—Se1	118.5 (5)	C17—C16—C15	119.8 (7)
C6—C1—Se1	121.8 (4)	C17—C16—H16	120.1
C1—C2—C3	121.1 (6)	C15—C16—H16	120.1
C1—C2—H2	119.4	C16—C17—C18	119.9 (6)
C3—C2—H2	119.4	C16—C17—H17	120.0
C4—C3—C2	117.9 (6)	C18—C17—H17	120.0
C4—C3—C7	120.9 (7)	C19—C18—C17	120.0 (6)
C2—C3—C7	121.1 (7)	C19—C18—H18	120.0
C3—C4—C5	121.5 (7)	C17—C18—H18	120.0
C3—C4—H4	119.3	C18—C19—C14	120.8 (6)
C5—C4—H4	119.3	C18—C19—H19	119.6
C6—C5—C4	120.4 (7)	C14—C19—H19	119.6
C6—C5—H5	119.8	C25—C20—C21	118.7 (6)
C4—C5—H5	119.8	C25—C20—Sn1	121.2 (4)
C5—C6—C1	119.4 (6)	C21—C20—Sn1	120.1 (4)
C5—C6—H6	120.3	C22—C21—C20	119.3 (6)
C1—C6—H6	120.3	C22—C21—H21	120.3
C3—C7—H7A	109.5	C20—C21—H21	120.3
C3—C7—H7B	109.5	C23—C22—C21	120.9 (7)
H7A—C7—H7B	109.5	C23—C22—H22	119.5
C3—C7—H7C	109.5	C21—C22—H22	119.5
H7A—C7—H7C	109.5	C22—C23—C24	120.2 (7)
H7B—C7—H7C	109.5	C22—C23—H23	119.9
C9—C8—C13	118.2 (5)	C24—C23—H23	119.9
C9—C8—Sn1	119.6 (4)	C23—C24—C25	120.3 (7)
C13—C8—Sn1	121.7 (4)	C23—C24—H24	119.9
C8—C9—C10	120.2 (6)	C25—C24—H24	119.9
C8—C9—H9	119.9	C20—C25—C24	120.6 (7)
C10—C9—H9	119.9	C20—C25—H25	119.7
C11—C10—C9	120.8 (7)	C24—C25—H25	119.7
C11—C10—H10	119.6		

Symmetry codes: (i) *x*, −*y*+1/2, *z*+1/2; (ii) *x*, −*y*+1/2, *z*−1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···O1	0.93	2.57	3.487 (7)	169.

Fig. 1

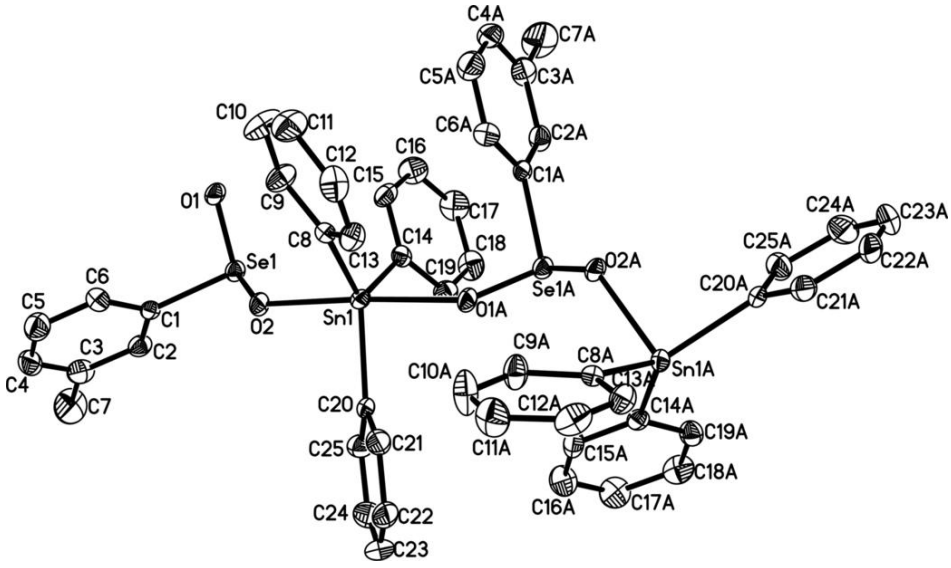
C4A
C7A
C5A
C3A
C10
C11
C6A
C2A
C12
C16
C15
C1A
O1
C9
C17
C24A
C23A
C8
C14
C18
C25A
Se1
C13
C19
O2A
C22A
C6
C20A
C5
C1
Se1A
C21A
O2
Sn1
O1A
C3
C2
C9A
C8A
C10A
Sn1A
C4
C13A
C12A
C14A
C7
C20
C19A
C25
C21
C11A
C15A
C18A
C24
C22
C16A
C17A
C23

Fig. 2