

Inorganic Chemistry

including bioinorganic chemistry

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Table 1. Crystal data and structure refinement for (OEC)Sn(C₆H₅).

Identification code	Phenyl(octaethylcorrolato)tin(IV)	
Empirical formula	C ₄₁ H ₄₈ N ₄ Sn	
Formula weight	715.52	
Temperature	293(2) K	
Wavelength, MoK α	0.71069 Å	
Crystal system	monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	a = 13.235(4) Å	alpha = 90 deg.
	b = 14.502(4) Å	beta = 95.45(2) deg.
	c = 18.387(5) Å	gamma = 90 deg.
Volume	3513(2) Å ³	
Z	4	
Density (calculated)	1.353 Mg/m ³	
Absorption coefficient	0.762 mm ⁻¹	
F(000)	1488	
Crystal form	needle	
Crystal size	0.35 x 0.30 x 0.28 mm	
Crystal color	red	
Theta range for data collection	1.79 to 23.94 deg.	
Index ranges	0 ≤ h ≤ 14, 0 ≤ k ≤ 15, -20 ≤ l ≤ 20	
Reflections collected	5541	
Independent reflections	5061	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4925 / 0 / 609	
Goodness-of-fit on F ²	1.087	
Weighting scheme calc	w = 1 / [s ² (Fo ²) + (0.0931P) ² + 5.3139P] where P = (Fo ² + 2Fc ²) / 3	
Final R indices [I > 2σ(I)]	R ₁ = 0.0619, wR ₂ = 0.1394	
Reflection observed	3845	
R indices (all data)	R ₁ = 0.0855, wR ₂ = 0.1686	
Largest diff. peak and hole	2.180 and -1.085 e.Å ⁻³	
Absorption correction:	PSI-Scan	
minimum transmission	59.16%	
maximum transmission	99.90%	
average transmission	78.53%	
maximum correction factor	0.9995	
average correction factor	0.8861	
Estimate of agreement between equivalent reflections	R _{sigma} = 0.056	
Scattering factors see:	SHELXL-93	

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Measurement made on ENRAF-NONIUS-CAD4-diffractometer, the structure was solved with direct methods and refined for all independent reflections against Fx₂ (heavy atoms with anisotropic, H atoms with isotropic temperature factors)

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for (OEC)Sn(C₆H₅). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Sn	2190(1)	4478(1)	8987(1)	30(1)
N(1)	1711(5)	5837(4)	8910(3)	36(1)
N(2)	1568(4)	4383(4)	7914(3)	33(1)
N(3)	1625(5)	3180(4)	9163(3)	36(1)
N(4)	1683(4)	4791(4)	9986(3)	34(1)
C(1)	1546(5)	6297(5)	9534(4)	38(2)
C(2)	1350(5)	7237(5)	9326(4)	38(2)
C(3)	1369(5)	7296(5)	8575(4)	39(2)
C(4)	1577(5)	6392(5)	8317(4)	37(2)
C(5)	1529(5)	6026(5)	7603(4)	36(2)
C(6)	1480(5)	5105(6)	7408(4)	39(2)
C(7)	1264(5)	4700(5)	6704(4)	37(2)
C(8)	1198(5)	3769(5)	6785(4)	38(2)
C(9)	1406(5)	3565(5)	7541(4)	34(2)
C(10)	1416(5)	2696(5)	7883(4)	36(2)
C(11)	1487(5)	2510(5)	8626(4)	33(2)
C(12)	1350(5)	1650(5)	8993(4)	40(2)
C(13)	1409(5)	1815(5)	9725(4)	37(2)
C(14)	1548(5)	2784(5)	9838(4)	35(2)
C(15)	1525(6)	3287(6)	10485(4)	42(2)
C(16)	1520(5)	4237(5)	10560(4)	37(2)
C(17)	1278(5)	4817(6)	11148(4)	39(2)
C(18)	1258(5)	5722(5)	10901(4)	37(2)
C(19)	1503(5)	5696(5)	10155(4)	37(2)
C(20)	1211(8)	8025(7)	9833(6)	53(2)
C(21)	2184(11)	8297(11)	10263(9)	95(5)
C(22)	1124(7)	8098(6)	8075(5)	49(2)
C(23)	43(8)	8115(8)	7742(6)	61(3)
C(24)	1063(7)	5274(7)	6025(5)	52(2)
C(25)	-9(10)	5681(9)	5935(7)	74(3)
C(26)	906(7)	3072(7)	6206(5)	53(2)
C(27)	-187(9)	2761(10)	6204(7)	80(3)
C(28)	1081(7)	760(5)	8596(5)	48(2)
C(29)	-22(9)	673(8)	8395(8)	75(3)
C(30)	1319(7)	1124(7)	10327(5)	49(2)
C(31)	2309(9)	903(9)	10749(7)	70(3)
C(32)	1067(7)	4459(7)	11881(5)	50(2)
C(33)	1996(12)	4192(11)	12349(7)	80(4)
C(34)	993(7)	6539(7)	11339(5)	52(2)
C(35)	1828(11)	6833(10)	11897(8)	90(4)
C(36)	3783(5)	4387(5)	9038(3)	31(2)
C(37)	4362(7)	5108(7)	8846(6)	68(3)
C(38)	5404(9)	5059(11)	8901(9)	94(5)
C(39)	5870(8)	4262(11)	9136(6)	83(4)
C(40)	5316(8)	3508(11)	9301(7)	91(4)
C(41)	4267(8)	3572(8)	9241(6)	69(3)

Table 3. Bond lengths [Å] and angles [deg] for (OEC)Sn(C₆H₅).

Sn-N(3)	2.062(6)
Sn-N(4)	2.065(5)
Sn-N(2)	2.069(6)
Sn-N(1)	2.072(6)
Sn-C(36)	2.105(7)
N(1)-C(4)	1.352(9)
N(1)-C(1)	1.363(9)
N(2)-C(9)	1.377(9)
N(2)-C(6)	1.399(9)
N(3)-C(14)	1.379(9)
N(3)-C(11)	1.386(9)
N(4)-C(16)	1.358(9)
N(4)-C(19)	1.375(9)
C(1)-C(2)	1.434(10)
C(1)-C(19)	1.442(10)
C(2)-C(3)	1.387(10)
C(2)-C(20)	1.497(12)
C(3)-C(4)	1.430(10)
C(3)-C(22)	1.498(11)
C(4)-C(5)	1.412(10)
C(5)-C(6)	1.382(11)
C(6)-C(7)	1.425(10)
C(7)-C(8)	1.363(10)
C(7)-C(24)	1.503(10)
C(8)-C(9)	1.422(10)
C(8)-C(26)	1.492(11)
C(9)-C(10)	1.408(10)
C(10)-C(11)	1.387(10)
C(11)-C(12)	1.437(10)
C(12)-C(13)	1.362(10)
C(12)-C(28)	1.508(11)
C(13)-C(14)	1.429(10)
C(13)-C(30)	1.507(11)
C(14)-C(15)	1.399(10)
C(15)-C(16)	1.386(11)
C(16)-C(17)	1.431(10)
C(17)-C(18)	1.389(11)
C(17)-C(32)	1.495(11)
C(18)-C(19)	1.439(10)
C(18)-C(34)	1.493(11)
C(20)-C(21)	1.50(2)
C(22)-C(23)	1.502(13)
C(24)-C(25)	1.53(2)
C(26)-C(27)	1.515(14)
C(28)-C(29)	1.477(14)
C(30)-C(31)	1.492(13)
C(32)-C(33)	1.48(2)
C(34)-C(35)	1.50(2)
C(36)-C(37)	1.362(12)
C(36)-C(41)	1.379(13)
C(37)-C(38)	1.38(2)
C(38)-C(39)	1.36(2)
C(39)-C(40)	1.37(2)
C(40)-C(41)	1.385(14)

N(3)-Sn-N(4)	84.7(2)	(OEC) Sn(C ₆ H ₅)
N(3)-Sn-N(2)	88.3(2)	
N(4)-Sn-N(2)	136.8(2)	
N(3)-Sn-N(1)	140.0(2)	
N(4)-Sn-N(1)	74.3(2)	
N(2)-Sn-N(1)	84.6(2)	
N(3)-Sn-C(36)	108.2(3)	
N(4)-Sn-C(36)	112.5(2)	
N(2)-Sn-C(36)	110.2(2)	
N(1)-Sn-C(36)	111.2(3)	
C(4)-N(1)-C(1)	111.7(6)	
C(4)-N(1)-Sn	129.6(5)	
C(1)-N(1)-Sn	118.7(5)	
C(9)-N(2)-C(6)	108.3(6)	
C(9)-N(2)-Sn	124.2(4)	
C(6)-N(2)-Sn	125.8(5)	
C(14)-N(3)-C(11)	109.5(6)	
C(14)-N(3)-Sn	125.4(5)	
C(11)-N(3)-Sn	123.6(4)	
C(16)-N(4)-C(19)	110.2(6)	
C(16)-N(4)-Sn	130.5(5)	
C(19)-N(4)-Sn	119.3(5)	
N(1)-C(1)-C(2)	106.2(6)	
N(1)-C(1)-C(19)	113.2(6)	
C(2)-C(1)-C(19)	140.0(7)	
C(3)-C(2)-C(1)	107.7(6)	
C(3)-C(2)-C(20)	126.1(8)	
C(1)-C(2)-C(20)	126.1(8)	
C(2)-C(3)-C(4)	107.2(6)	
C(2)-C(3)-C(22)	129.5(7)	
C(4)-C(3)-C(22)	123.1(7)	
N(1)-C(4)-C(5)	121.1(7)	
N(1)-C(4)-C(3)	107.1(6)	
C(5)-C(4)-C(3)	131.3(7)	
C(6)-C(5)-C(4)	127.0(7)	
C(5)-C(6)-N(2)	123.5(7)	
C(5)-C(6)-C(7)	129.3(7)	
N(2)-C(6)-C(7)	107.0(7)	
C(8)-C(7)-C(6)	108.6(6)	
C(8)-C(7)-C(24)	129.1(7)	
C(6)-C(7)-C(24)	122.1(7)	
C(7)-C(8)-C(9)	107.8(6)	
C(7)-C(8)-C(26)	127.5(7)	
C(9)-C(8)-C(26)	124.7(7)	
N(2)-C(9)-C(10)	123.6(6)	
N(2)-C(9)-C(8)	108.3(6)	
C(10)-C(9)-C(8)	128.0(7)	
C(11)-C(10)-C(9)	127.7(7)	
N(3)-C(11)-C(10)	123.9(6)	
N(3)-C(11)-C(12)	106.7(6)	
C(10)-C(11)-C(12)	129.2(7)	
C(13)-C(12)-C(11)	108.3(6)	
C(13)-C(12)-C(28)	128.1(7)	
C(11)-C(12)-C(28)	123.3(7)	
C(12)-C(13)-C(14)	108.1(6)	
C(12)-C(13)-C(30)	127.5(7)	
C(14)-C(13)-C(30)	124.4(7)	
N(3)-C(14)-C(15)	123.9(7)	

		(OEC) Sn(C ₆ H ₅)
N(3)-C(14)-C(13)	107.3(6)	
C(15)-C(14)-C(13)	128.5(7)	
C(16)-C(15)-C(14)	127.1(7)	
N(4)-C(16)-C(15)	120.6(7)	
N(4)-C(16)-C(17)	107.6(6)	
C(15)-C(16)-C(17)	131.5(7)	
C(18)-C(17)-C(16)	107.8(6)	
C(18)-C(17)-C(32)	128.6(7)	
C(16)-C(17)-C(32)	123.5(7)	
C(17)-C(18)-C(19)	106.7(6)	
C(17)-C(18)-C(34)	124.8(7)	
C(19)-C(18)-C(34)	128.4(7)	
N(4)-C(19)-C(18)	107.5(6)	
N(4)-C(19)-C(1)	112.2(6)	
C(18)-C(19)-C(1)	140.2(7)	
C(2)-C(20)-C(21)	112.2(9)	
C(3)-C(22)-C(23)	113.9(7)	
C(7)-C(24)-C(25)	113.1(8)	
C(8)-C(26)-C(27)	112.7(7)	
C(29)-C(28)-C(12)	112.1(7)	
C(31)-C(30)-C(13)	113.4(8)	
C(33)-C(32)-C(17)	113.4(9)	
C(18)-C(34)-C(35)	113.6(8)	
C(37)-C(36)-C(41)	118.0(8)	
C(37)-C(36)-Sn	121.7(6)	
C(41)-C(36)-Sn	120.2(6)	
C(36)-C(37)-C(38)	121.7(12)	
C(39)-C(38)-C(37)	119.3(13)	
C(40)-C(39)-C(38)	120.9(10)	
C(39)-C(40)-C(41)	118.9(12)	
C(40)-C(41)-C(36)	121.0(12)	

Table 4. Torsion angles [deg] for (OEC)Sn(C₆H₅).

N(3)-Sn-N(1)-C(4)	-108.8(6)
N(4)-Sn-N(1)-C(4)	-169.8(7)
N(2)-Sn-N(1)-C(4)	-27.8(6)
C(36)-Sn-N(1)-C(4)	81.7(7)
N(3)-Sn-N(1)-C(1)	75.3(6)
N(4)-Sn-N(1)-C(1)	14.3(5)
N(2)-Sn-N(1)-C(1)	156.3(6)
C(36)-Sn-N(1)-C(1)	-94.2(5)
N(3)-Sn-N(2)-C(9)	-27.5(5)
N(4)-Sn-N(2)-C(9)	-108.0(5)
N(1)-Sn-N(2)-C(9)	-168.1(5)
C(36)-Sn-N(2)-C(9)	81.3(6)
N(3)-Sn-N(2)-C(6)	169.2(5)
N(4)-Sn-N(2)-C(6)	88.7(6)
N(1)-Sn-N(2)-C(6)	28.6(5)
C(36)-Sn-N(2)-C(6)	-82.0(6)
N(4)-Sn-N(3)-C(14)	-28.6(6)
N(2)-Sn-N(3)-C(14)	-165.9(6)
N(1)-Sn-N(3)-C(14)	-86.3(7)
C(36)-Sn-N(3)-C(14)	83.4(6)
N(4)-Sn-N(3)-C(11)	166.9(6)
N(2)-Sn-N(3)-C(11)	29.6(5)
N(1)-Sn-N(3)-C(11)	109.2(6)
C(36)-Sn-N(3)-C(11)	-81.1(6)
N(3)-Sn-N(4)-C(16)	24.7(6)
N(2)-Sn-N(4)-C(16)	106.6(6)
N(1)-Sn-N(4)-C(16)	170.3(7)
C(36)-Sn-N(4)-C(16)	-82.8(7)
N(3)-Sn-N(4)-C(19)	-158.4(6)
N(2)-Sn-N(4)-C(19)	-76.5(6)
N(1)-Sn-N(4)-C(19)	-12.8(5)
C(36)-Sn-N(4)-C(19)	94.1(6)
C(4)-N(1)-C(1)-C(2)	-3.6(8)
Sn-N(1)-C(1)-C(2)	172.9(4)
C(4)-N(1)-C(1)-C(19)	169.6(6)
Sn-N(1)-C(1)-C(19)	-13.8(8)
N(1)-C(1)-C(2)-C(3)	2.1(8)
C(19)-C(1)-C(2)-C(3)	-168.1(9)
N(1)-C(1)-C(2)-C(20)	-174.6(7)
C(19)-C(1)-C(2)-C(20)	15.2(14)
C(1)-C(2)-C(3)-C(4)	.0(8)
C(20)-C(2)-C(3)-C(4)	176.7(7)
C(1)-C(2)-C(3)-C(22)	174.1(8)
C(20)-C(2)-C(3)-C(22)	-9.2(13)
C(1)-N(1)-C(4)-C(5)	-168.5(6)
Sn-N(1)-C(4)-C(5)	15.4(10)
C(1)-N(1)-C(4)-C(3)	3.7(8)
Sn-N(1)-C(4)-C(3)	-172.4(5)
C(2)-C(3)-C(4)-N(1)	-2.2(8)
C(22)-C(3)-C(4)-N(1)	-176.7(7)
C(2)-C(3)-C(4)-C(5)	168.9(7)
C(22)-C(3)-C(4)-C(5)	-5.6(12)
N(1)-C(4)-C(5)-C(6)	8.6(12)
C(3)-C(4)-C(5)-C(6)	-161.5(8)

C(4)-C(5)-C(6)-N(2)	-6.2(12)
C(4)-C(5)-C(6)-C(7)	168.5(7)
C(9)-N(2)-C(6)-C(5)	175.3(7)
Sn-N(2)-C(6)-C(5)	-19.2(9)
C(9)-N(2)-C(6)-C(7)	-.4(7)
Sn-N(2)-C(6)-C(7)	165.1(4)
C(5)-C(6)-C(7)-C(8)	-173.9(7)
N(2)-C(6)-C(7)-C(8)	1.5(8)
C(5)-C(6)-C(7)-C(24)	1.2(12)
N(2)-C(6)-C(7)-C(24)	176.6(7)
C(6)-C(7)-C(8)-C(9)	-1.9(8)
C(24)-C(7)-C(8)-C(9)	-176.6(7)
C(6)-C(7)-C(8)-C(26)	174.9(7)
C(24)-C(7)-C(8)-C(26)	.2(13)
C(6)-N(2)-C(9)-C(10)	-178.7(6)
Sn-N(2)-C(9)-C(10)	15.6(9)
C(6)-N(2)-C(9)-C(8)	-.8(7)
Sn-N(2)-C(9)-C(8)	-166.6(4)
C(7)-C(8)-C(9)-N(2)	1.7(8)
C(26)-C(8)-C(9)-N(2)	-175.2(7)
C(7)-C(8)-C(9)-C(10)	179.5(7)
C(26)-C(8)-C(9)-C(10)	2.5(12)
N(2)-C(9)-C(10)-C(11)	6.7(11)
C(8)-C(9)-C(10)-C(11)	-170.7(7)
C(14)-N(3)-C(11)-C(10)	173.3(7)
Sn-N(3)-C(11)-C(10)	-20.0(9)
C(14)-N(3)-C(11)-C(12)	-1.9(8)
Sn-N(3)-C(11)-C(12)	164.8(5)
C(9)-C(10)-C(11)-N(3)	-4.3(12)
C(9)-C(10)-C(11)-C(12)	169.8(7)
N(3)-C(11)-C(12)-C(13)	-.1(8)
C(10)-C(11)-C(12)-C(13)	-174.9(7)
N(3)-C(11)-C(12)-C(28)	174.2(7)
C(10)-C(11)-C(12)-C(28)	-.7(12)
C(11)-C(12)-C(13)-C(14)	2.0(8)
C(28)-C(12)-C(13)-C(14)	-171.9(7)
C(11)-C(12)-C(13)-C(30)	-179.6(7)
C(28)-C(12)-C(13)-C(30)	6.5(13)
C(11)-N(3)-C(14)-C(15)	-171.8(7)
Sn-N(3)-C(14)-C(15)	21.8(10)
C(11)-N(3)-C(14)-C(13)	3.1(8)
Sn-N(3)-C(14)-C(13)	-163.3(5)
C(12)-C(13)-C(14)-N(3)	-3.1(8)
C(30)-C(13)-C(14)-N(3)	178.4(7)
C(12)-C(13)-C(14)-C(15)	171.5(7)
C(30)-C(13)-C(14)-C(15)	-7.0(13)
N(3)-C(14)-C(15)-C(16)	3.6(13)
C(13)-C(14)-C(15)-C(16)	-170.2(8)
C(19)-N(4)-C(16)-C(15)	171.5(7)
Sn-N(4)-C(16)-C(15)	-11.3(10)
C(19)-N(4)-C(16)-C(17)	-3.5(8)
Sn-N(4)-C(16)-C(17)	173.6(5)
C(14)-C(15)-C(16)-N(4)	-9.4(12)
C(14)-C(15)-C(16)-C(17)	164.3(8)
N(4)-C(16)-C(17)-C(18)	2.6(8)
C(15)-C(16)-C(17)-C(18)	-171.7(8)
N(4)-C(16)-C(17)-C(32)	-178.9(7)
C(15)-C(16)-C(17)-C(32)	6.9(13)

(OEC) Sn(C₆H₅)

C(16)-C(17)-C(18)-C(19)	-0.7(8)	(OEC) Sn(C ₆ H ₅)
C(32)-C(17)-C(18)-C(19)	-179.2(8)	
C(16)-C(17)-C(18)-C(34)	177.4(7)	
C(32)-C(17)-C(18)-C(34)	-1.0(13)	
C(16)-N(4)-C(19)-C(18)	3.1(8)	
Sn-N(4)-C(19)-C(18)	-174.4(4)	
C(16)-N(4)-C(19)-C(1)	-173.0(6)	
Sn-N(4)-C(19)-C(1)	9.5(8)	
C(17)-C(18)-C(19)-N(4)	-1.4(8)	
C(34)-C(18)-C(19)-N(4)	-179.4(7)	
C(17)-C(18)-C(19)-C(1)	172.9(9)	
C(34)-C(18)-C(19)-C(1)	-5(2)	
N(1)-C(1)-C(19)-N(4)	2.7(9)	
C(2)-C(1)-C(19)-N(4)	172.5(8)	
N(1)-C(1)-C(19)-C(18)	-171.4(9)	
C(2)-C(1)-C(19)-C(18)	-2(2)	
C(3)-C(2)-C(20)-C(21)	-104.6(12)	
C(1)-C(2)-C(20)-C(21)	71.5(13)	
C(2)-C(3)-C(22)-C(23)	-93.4(11)	
C(4)-C(3)-C(22)-C(23)	79.8(11)	
C(8)-C(7)-C(24)-C(25)	96.3(11)	
C(6)-C(7)-C(24)-C(25)	-77.8(11)	
C(7)-C(8)-C(26)-C(27)	-100.3(11)	
C(9)-C(8)-C(26)-C(27)	76.0(12)	
C(13)-C(12)-C(28)-C(29)	89.4(12)	
C(11)-C(12)-C(28)-C(29)	-83.7(11)	
C(12)-C(13)-C(30)-C(31)	105.8(11)	
C(14)-C(13)-C(30)-C(31)	-76.0(11)	
C(18)-C(17)-C(32)-C(33)	-104.4(11)	
C(16)-C(17)-C(32)-C(33)	77.4(12)	
C(17)-C(18)-C(34)-C(35)	76.7(13)	
C(19)-C(18)-C(34)-C(35)	-105.6(12)	
N(3)-Sn-C(36)-C(37)	171.0(7)	
N(4)-Sn-C(36)-C(37)	-97.2(7)	
N(2)-Sn-C(36)-C(37)	75.9(7)	
N(1)-Sn-C(36)-C(37)	-16.1(8)	
N(3)-Sn-C(36)-C(41)	-6.3(7)	
N(4)-Sn-C(36)-C(41)	85.5(7)	
N(2)-Sn-C(36)-C(41)	-101.4(7)	
N(1)-Sn-C(36)-C(41)	166.6(7)	
C(41)-C(36)-C(37)-C(38)	-5(2)	
Sn-C(36)-C(37)-C(38)	178.0(9)	
C(36)-C(37)-C(38)-C(39)	2(2)	
C(37)-C(38)-C(39)-C(40)	2(2)	
C(38)-C(39)-C(40)-C(41)	-2(2)	
C(39)-C(40)-C(41)-C(36)	-2(2)	
C(37)-C(36)-C(41)-C(40)	5(2)	
Sn-C(36)-C(41)-C(40)	-177.9(8)	

Table 5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (OEC)Sn(C₆H₅). The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Sn	31(1)	27(1)	32(1)	0(1)	2(1)	0(1)
N(1)	48(4)	24(3)	37(3)	4(3)	6(3)	6(3)
N(2)	32(3)	34(3)	34(3)	7(3)	1(2)	3(3)
N(3)	49(4)	34(3)	26(3)	1(3)	2(3)	0(3)
N(4)	45(4)	27(3)	30(3)	-2(3)	6(3)	7(3)
C(1)	30(4)	39(4)	45(4)	-6(4)	3(3)	2(3)
C(2)	31(4)	29(4)	54(5)	-9(3)	3(3)	-6(3)
C(3)	34(4)	31(4)	50(5)	2(3)	-4(3)	-4(3)
C(4)	32(4)	37(4)	39(4)	4(3)	-3(3)	-1(3)
C(5)	36(4)	31(4)	42(4)	10(4)	0(3)	-2(3)
C(6)	32(4)	51(5)	35(4)	10(4)	4(3)	1(3)
C(7)	40(4)	44(5)	25(4)	4(3)	2(3)	0(3)
C(8)	30(4)	47(5)	36(4)	-5(3)	4(3)	1(3)
C(9)	32(4)	34(4)	37(4)	-1(3)	5(3)	2(3)
C(10)	37(4)	31(4)	41(4)	-12(4)	8(3)	-2(3)
C(11)	36(4)	28(4)	35(4)	-4(3)	7(3)	3(3)
C(12)	32(4)	38(5)	51(5)	-3(4)	6(3)	2(3)
C(13)	37(4)	28(4)	47(5)	4(3)	9(3)	2(3)
C(14)	40(4)	26(4)	37(4)	4(3)	3(3)	-4(3)
C(15)	49(5)	41(5)	38(4)	14(4)	9(4)	2(4)
C(16)	32(4)	36(5)	41(4)	2(3)	1(3)	-6(3)
C(17)	29(4)	49(5)	41(4)	-6(4)	3(3)	0(3)
C(18)	33(4)	38(5)	40(4)	-11(3)	-1(3)	6(3)
C(19)	33(4)	33(4)	46(4)	1(3)	1(3)	4(3)
C(20)	58(6)	35(5)	67(7)	8(5)	13(5)	3(4)
C(21)	89(9)	98(10)	101(10)	-68(9)	19(8)	-19(8)
C(22)	61(6)	29(5)	57(5)	8(4)	5(5)	1(4)
C(23)	78(7)	42(6)	62(6)	19(5)	4(5)	12(5)
C(24)	71(6)	50(6)	33(5)	4(4)	2(4)	7(5)
C(25)	96(9)	64(8)	55(7)	8(6)	-20(6)	6(6)
C(26)	64(6)	53(6)	42(5)	-1(4)	8(4)	4(5)
C(27)	63(7)	97(10)	76(8)	-37(7)	-8(6)	-1(6)
C(28)	63(6)	23(4)	60(6)	-3(4)	13(5)	0(4)
C(29)	69(7)	56(7)	99(9)	-28(7)	7(7)	-16(5)
C(30)	54(5)	36(5)	56(5)	1(4)	3(4)	0(4)
C(31)	72(7)	53(7)	82(7)	29(6)	-13(6)	6(6)
C(32)	56(5)	49(5)	49(5)	2(4)	17(4)	-4(5)
C(33)	92(9)	97(10)	51(6)	23(6)	1(6)	7(8)
C(34)	58(6)	47(6)	50(5)	-7(5)	7(4)	9(5)
C(35)	113(11)	69(9)	86(9)	-48(8)	3(8)	-3(8)
C(36)	29(4)	40(4)	24(3)	0(3)	0(3)	3(3)
C(37)	34(5)	55(6)	115(9)	-12(6)	11(5)	-2(5)
C(38)	52(7)	80(9)	154(13)	-37(9)	30(8)	-18(7)
C(39)	35(6)	141(13)	72(7)	-48(8)	-3(5)	0(7)
C(40)	39(6)	128(11)	104(9)	6(8)	0(5)	35(7)
C(41)	58(6)	76(8)	72(7)	12(6)	4(5)	17(5)

Table 6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (OEC)Sn(C₆H₅).

	x	y	z	U(eq)
H(5)	1504(54)	6448(55)	7241(41)	43(22)
H(10)	1378(38)	2204(40)	7573(29)	6(13)
H(15)	1418(46)	2932(46)	10812(35)	19(17)
H(20A)	726(63)	7928(56)	10143(44)	53(24)
H(20B)	1035(44)	8346(45)	9573(33)	6(18)
H(21A)	2112(64)	8613(65)	10589(49)	48(27)
H(21B)	2636(75)	8549(68)	9858(56)	81(32)
H(21C)	2655(110)	7784(105)	10567(79)	148(63)
H(22A)	1519(76)	8014(70)	7693(56)	84(34)
H(22B)	1298(63)	8609(66)	8375(47)	62(27)
H(23A)	-145(52)	8606(55)	7465(39)	34(20)
H(23B)	-418(67)	8162(59)	8102(48)	61(27)
H(23C)	-101(52)	7522(58)	7562(38)	34(20)
H(24A)	1222(44)	4869(45)	5697(34)	13(16)
H(24B)	1424(65)	5891(65)	6044(45)	63(26)
H(25A)	-76(88)	5900(83)	5552(67)	95(44)
H(25B)	-31(75)	6057(74)	6361(61)	82(35)
H(25C)	-475(66)	5123(67)	5917(45)	58(26)
H(26A)	959(66)	3380(65)	5814(50)	64(29)
H(26B)	1366(55)	2537(55)	6334(38)	36(20)
H(27A)	-472(64)	2502(62)	5727(50)	60(25)
H(27B)	-624(95)	3339(93)	6220(67)	127(46)
H(27C)	-430(70)	2541(67)	6681(55)	73(31)
H(28A)	1438(66)	739(57)	8178(50)	59(26)
H(28B)	1393(51)	251(52)	8879(37)	31(19)
H(29A)	-88(73)	90(80)	8072(56)	86(31)
H(29B)	-230(71)	1153(73)	8028(53)	73(33)
H(29C)	-420(93)	597(73)	8798(68)	95(41)
H(30A)	835(67)	1382(64)	10629(49)	67(27)
H(30B)	1145(64)	635(62)	10109(47)	52(26)
H(31A)	2289(62)	409(59)	11094(46)	52(23)
H(31B)	2567(61)	1419(67)	10996(43)	51(26)
H(31C)	2957(87)	657(70)	10522(58)	90(35)
H(32A)	667(64)	4848(62)	12024(46)	51(27)
H(32B)	540(54)	3940(52)	11758(37)	37(19)
H(33A)	1741(104)	3984(101)	12682(80)	121(54)
H(33B)	2583(129)	4583(109)	12411(87)	146(67)
H(33C)	2478(114)	3690(113)	12036(81)	159(58)
H(34A)	824(68)	6980(68)	11072(49)	61(30)
H(34B)	433(72)	6276(67)	11600(51)	78(30)
H(35A)	1742(52)	7253(54)	12236(40)	35(19)
H(35B)	2446(69)	7050(59)	11656(46)	60(28)
H(35C)	2013(88)	6307(91)	12128(63)	98(47)
H(37)	4051(75)	5616(63)	8747(53)	69(31)
H(38)	5616(114)	5493(91)	8711(80)	120(58)
H(39)	6657(89)	4331(66)	9133(55)	87(32)
H(40)	5618(84)	2831(80)	9501(59)	100(37)
H(41)	3924(121)	3207(116)	9433(86)	177(72)