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Crystal Structures of μ_2 -Fluoro- and μ_2 -Salicylaldoximate-Bridged μ_3 -Oxo-Tris(Dimethyltin(IV)) Bis(Salicylaldoximate)

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- SUPPLEMENTARY MATERIAL -

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* Table available from the authors

N.B. CIF document is available from etiekink@chemistry.adelaide.edu.au

Table S(1) **Fractional atomic coordinates for [C₂₀H₂₉FN₂O₆Sn₃]**

Atom	x	y	z	B(eq) ^a
Sn(1)	0.05032(5)	0.10279(3)	0.18546(8)	1.99(2)
Sn(2)	-0.11449(6)	0.03734(3)	0.29390(8)	2.12(2)
Sn(3)	-0.13173(6)	0.16687(4)	0.2556(1)	3.22(2)
F(40)	-0.2001(4)	0.1003(3)	0.3107(7)	3.2(2)
O(9)	0.2135(6)	0.0454(3)	0.1373(9)	3.4(2)
O(10)	-0.0050(5)	0.0098(3)	0.2604(8)	2.6(2)
O(19)	-0.0404(6)	0.2130(3)	0.2144(8)	3.2(2)
O(20)	0.1505(5)	0.1375(3)	0.1135(8)	2.8(2)
O(30)	-0.0642(5)	0.1051(3)	0.2542(7)	2.2(2)
N(8)	0.1451(6)	0.0272(4)	0.1748(9)	2.4(3)
N(18)	0.0152(7)	0.1885(4)	0.150(1)	2.7(3)
C(1)	0.0880(8)	-0.0575(4)	0.232(1)	2.2(3)
C(2)	0.0157(8)	-0.0416(5)	0.267(1)	2.2(3)
C(3)	-0.0339(9)	-0.0803(5)	0.303(1)	3.3(4)
C(4)	-0.014(1)	-0.1319(5)	0.309(1)	3.7(4)
C(5)	0.055(1)	-0.1476(5)	0.277(1)	3.8(4)
C(6)	0.1031(9)	-0.1107(5)	0.237(1)	2.9(3)
C(7)	0.1461(8)	-0.0225(5)	0.192(1)	2.6(3)
C(11)	0.0983(8)	0.2018(5)	-0.015(1)	2.8(3)
C(12)	0.1521(8)	0.1624(5)	0.008(1)	2.4(3)
C(13)	0.2059(9)	0.1517(5)	-0.072(1)	3.1(4)
C(14)	0.211(1)	0.1795(6)	-0.176(2)	4.7(5)
C(15)	0.158(1)	0.2177(6)	-0.203(1)	4.1(4)
C(16)	0.1051(10)	0.2291(5)	-0.124(1)	3.2(4)
C(17)	0.0410(9)	0.2162(5)	0.062(1)	2.8(3)
C(21)	0.0114(8)	0.0756(5)	0.022(1)	2.7(3)
C(22)	0.0911(9)	0.1127(5)	0.356(1)	3.5(4)
C(23)	-0.1214(9)	0.0253(5)	0.476(1)	3.3(4)
C(24)	-0.1718(9)	0.0036(5)	0.150(1)	3.3(4)
C(25)	-0.189(1)	0.1747(8)	0.101(2)	9.8(8)
C(26)	-0.149(1)	0.2053(7)	0.415(2)	10.9(9)
H(3)	-0.0830	-0.0704	0.3242	3.9206
H(4)	-0.0491	-0.1571	0.3353	4.4839
H(5)	0.0688	-0.1835	0.2825	4.5384
H(6)	0.1506	-0.1223	0.2119	3.4962

H(7)	0.1924	-0.0390	0.1763	3.1186
H(9)	0.2203	0.0817	0.1213	4.0717
H(13)	0.2408	0.1245	-0.0566	3.7699
H(14)	0.2505	0.1725	-0.2285	5.5852
H(15)	0.1598	0.2355	-0.2763	4.9385
H(16)	0.0708	0.2564	-0.1405	3.8116
H(17)	0.0185	0.2495	0.0486	3.3142
H(21a)	-0.0215	0.1008	-0.0109	3.1817
H(21b)	0.0524	0.0704	-0.0293	3.1817
H(21c)	-0.0142	0.0432	0.0321	3.1817
H(22a)	0.0748	0.0843	0.4034	4.1473
H(22b)	0.1439	0.1134	0.3542	4.1473
H(22c)	0.0731	0.1449	0.3871	4.1473
H(23a)	-0.1088	0.0569	0.5156	3.9588
H(23b)	-0.1707	0.0153	0.4963	3.9588
H(23c)	-0.0879	-0.0017	0.4985	3.9588
H(24a)	-0.2201	-0.0069	0.1735	3.9841
H(24b)	-0.1757	0.0289	0.0888	3.9841
H(24c)	-0.1451	-0.0261	0.1221	3.9841
H(25a)	-0.1992	0.2108	0.0868	11.7773
H(25b)	-0.1603	0.1609	0.0387	11.7773
H(25c)	-0.2349	0.1560	0.1059	11.7773
H(26a)	-0.1059	0.2014	0.4625	13.1141
H(26b)	-0.1576	0.2416	0.4009	13.1141
H(26c)	-0.1906	0.1904	0.4533	13.1141

$$a B_{eq} = (8\pi^2/3)(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma +$$

$$2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table S(2) Anisotropic thermal parameters ($\text{\AA}^2$) for $[\text{C}_{20}\text{H}_{29}\text{FN}_2\text{O}_6\text{Sn}_3]$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn(1)	0.0255(5)	0.0276(4)	0.0225(5)	-0.0007(4)	-0.0014(4)	0.0000(4)
Sn(2)	0.0278(6)	0.0301(5)	0.0228(5)	-0.0025(4)	-0.0001(4)	0.0005(4)
Sn(3)	0.0338(6)	0.0295(5)	0.0591(7)	0.0050(4)	0.0103(6)	0.0025(5)
F(40)	0.027(5)	0.045(4)	0.048(5)	-0.004(4)	0.013(4)	0.002(4)
O(9)	0.030(6)	0.034(5)	0.066(7)	0.004(4)	0.008(5)	0.013(5)
O(10)	0.032(6)	0.032(5)	0.033(6)	0.000(4)	0.007(5)	-0.006(4)
O(19)	0.052(8)	0.025(4)	0.045(6)	0.000(4)	0.021(6)	-0.006(4)
O(20)	0.026(6)	0.042(5)	0.040(6)	-0.002(4)	-0.001(5)	0.023(5)
O(30)	0.030(6)	0.023(4)	0.030(5)	-0.002(4)	0.012(5)	0.003(4)
N(8)	0.030(7)	0.040(6)	0.023(6)	-0.002(5)	0.004(5)	0.003(5)
N(18)	0.033(8)	0.028(6)	0.040(7)	-0.006(5)	-0.004(6)	-0.002(5)
C(1)	0.046(10)	0.023(6)	0.014(7)	0.011(6)	-0.001(6)	0.003(5)
C(2)	0.030(9)	0.032(7)	0.020(7)	-0.003(6)	-0.002(6)	0.002(6)
C(3)	0.06(1)	0.039(7)	0.029(8)	-0.003(7)	0.005(8)	-0.001(7)
C(4)	0.08(1)	0.019(7)	0.045(10)	-0.006(7)	-0.006(10)	0.013(7)
C(5)	0.06(1)	0.031(8)	0.05(1)	0.004(8)	0.005(10)	-0.006(7)
C(6)	0.05(1)	0.032(7)	0.031(8)	0.000(7)	-0.003(8)	-0.003(6)
C(7)	0.037(9)	0.043(8)	0.019(7)	0.021(7)	-0.008(7)	-0.007(6)
C(11)	0.04(1)	0.026(7)	0.041(9)	-0.009(6)	-0.004(8)	0.004(6)
C(12)	0.021(8)	0.026(6)	0.043(9)	-0.006(6)	0.003(7)	0.006(6)
C(13)	0.038(10)	0.041(8)	0.040(9)	0.003(7)	0.016(8)	0.012(7)
C(14)	0.05(1)	0.06(1)	0.07(1)	0.012(9)	0.02(1)	0.009(9)
C(15)	0.06(1)	0.06(1)	0.04(1)	0.004(8)	0.011(9)	0.020(8)
C(16)	0.05(1)	0.041(8)	0.027(8)	-0.004(7)	-0.005(8)	0.008(6)
C(17)	0.04(1)	0.026(7)	0.038(9)	0.006(6)	0.014(8)	-0.002(6)
C(21)	0.05(1)	0.028(7)	0.021(7)	0.006(6)	-0.011(7)	-0.008(6)
C(22)	0.04(1)	0.044(9)	0.05(1)	-0.021(7)	-0.007(8)	0.009(7)
C(23)	0.04(1)	0.050(9)	0.031(8)	0.001(8)	0.000(8)	0.000(7)
C(24)	0.04(1)	0.046(8)	0.039(9)	-0.006(7)	0.007(8)	-0.009(7)
C(25)	0.10(2)	0.12(2)	0.15(2)	-0.02(1)	-0.05(2)	0.10(2)
C(26)	0.16(3)	0.07(1)	0.19(3)	-0.07(1)	0.13(2)	-0.08(2)

where the anisotropic thermal parameter is given by the expression:

$$T_{\text{aniso}} = \exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^{*}b^{*}U_{12} + 2hla^{*}c^{*}U_{13} + 2klb^{*}c^{*}U_{23})].$$

Table S(3) **All bond distances (Å) for [C₂₀H₂₉FN₂O₆Sn₃]**

atom	atom	distance	atom	atom	distance
Sn(1)	O(10)	2.706(8)	O(19)	N(18)	1.39(1)
Sn(1)	O(20)	2.169(9)	O(20)	C(12)	1.37(2)
Sn(1)	O(30)	2.207(9)	N(8)	C(7)	1.28(2)
Sn(1)	N(8)	2.57(1)	N(18)	C(17)	1.32(2)
Sn(1)	N(18)	2.31(1)	C(1)	C(2)	1.42(2)
Sn(1)	C(21)	2.12(1)	C(1)	C(6)	1.38(2)
Sn(1)	C(22)	2.10(2)	C(1)	C(7)	1.45(2)
Sn(2)	F(40)	2.231(8)	C(2)	C(3)	1.39(2)
Sn(2)	O(10)	2.126(9)	C(3)	C(4)	1.36(2)
Sn(2)	O(30)	1.998(8)	C(4)	C(5)	1.35(2)
Sn(2)	C(23)	2.11(1)	C(5)	C(6)	1.36(2)
Sn(2)	C(24)	2.13(1)	C(11)	C(12)	1.42(2)
Sn(3)	F(40)	2.185(7)	C(11)	C(16)	1.42(2)
Sn(3)	O(19)	2.07(1)	C(11)	C(17)	1.41(2)
Sn(3)	O(30)	1.986(8)	C(12)	C(13)	1.36(2)
Sn(3)	C(25)	2.06(2)	C(13)	C(14)	1.39(2)
Sn(3)	C(26)	2.09(2)	C(14)	C(15)	1.39(2)
O(9)	N(8)	1.38(1)	C(15)	C(16)	1.35(2)
O(10)	C(2)	1.36(1)			

Table S(4) All bond angles (°) for [C₂₀H₂₉FN₂O₆Sn₃]

atom	atom	atom	angle	atom	atom	atom	angle
O(10)	Sn(1)	O(20)	141.4(3)	O(10)	Sn(2)	C(23)	100.7(5)
O(10)	Sn(1)	O(30)	64.3(3)	O(10)	Sn(2)	C(24)	100.1(5)
O(10)	Sn(1)	N(8)	66.7(3)	O(30)	Sn(2)	C(23)	112.1(4)
O(10)	Sn(1)	N(18)	141.4(4)	O(30)	Sn(2)	C(24)	113.0(5)
O(10)	Sn(1)	C(21)	82.7(4)	C(23)	Sn(2)	C(24)	132.8(6)
O(10)	Sn(1)	C(22)	86.5(4)	F(40)	Sn(3)	O(19)	161.8(3)
O(20)	Sn(1)	O(30)	154.2(3)	F(40)	Sn(3)	O(30)	74.6(3)
O(20)	Sn(1)	N(8)	74.7(3)	F(40)	Sn(3)	C(25)	92.3(6)
O(20)	Sn(1)	N(18)	77.1(4)	F(40)	Sn(3)	C(26)	91.6(5)
O(20)	Sn(1)	C(21)	94.1(5)	O(19)	Sn(3)	O(30)	87.8(3)
O(20)	Sn(1)	C(22)	90.8(5)	O(19)	Sn(3)	C(25)	98.5(7)
O(30)	Sn(1)	N(8)	131.0(3)	O(19)	Sn(3)	C(26)	92.9(6)
O(30)	Sn(1)	N(18)	77.3(4)	O(30)	Sn(3)	C(25)	112.1(8)
O(30)	Sn(1)	C(21)	90.9(5)	O(30)	Sn(3)	C(26)	117.8(9)
O(30)	Sn(1)	C(22)	89.5(5)	C(25)	Sn(3)	C(26)	129(1)
N(8)	Sn(1)	N(18)	151.7(4)	Sn(2)	F(40)	Sn(3)	98.2(3)
N(8)	Sn(1)	C(21)	86.1(4)	Sn(1)	O(10)	Sn(2)	96.3(3)
N(8)	Sn(1)	C(22)	84.4(5)	Sn(1)	O(10)	C(2)	139.3(8)
N(18)	Sn(1)	C(21)	93.7(4)	Sn(2)	O(10)	C(2)	124.0(8)
N(18)	Sn(1)	C(22)	98.3(5)	Sn(3)	O(19)	N(18)	115.9(6)
C(21)	Sn(1)	C(22)	167.8(5)	Sn(1)	O(20)	C(12)	122.9(8)
F(40)	Sn(2)	O(10)	153.2(3)	Sn(1)	O(30)	Sn(2)	118.7(4)
F(40)	Sn(2)	O(30)	73.3(3)	Sn(1)	O(30)	Sn(3)	126.5(4)
F(40)	Sn(2)	C(23)	88.7(4)	Sn(2)	O(30)	Sn(3)	113.8(4)
F(40)	Sn(2)	C(24)	91.3(5)	Sn(1)	N(8)	O(9)	110.7(7)
O(10)	Sn(2)	O(30)	79.9(3)	Sn(1)	N(8)	C(7)	137.8(9)
O(9)	N(8)	C(7)	111(1)				
Sn(1)	N(18)	O(19)	122.0(7)				
Sn(1)	N(18)	C(17)	122.8(9)				
O(19)	N(18)	C(17)	115(1)				
C(2)	C(1)	C(6)	116(1)				
C(2)	C(1)	C(7)	125(1)				
C(6)	C(1)	C(7)	119(1)				
O(10)	C(2)	C(1)	120(1)				
O(10)	C(2)	C(3)	121(1)				

C(1)	C(2)	C(3)	118(1)
C(2)	C(3)	C(4)	122(2)
C(3)	C(4)	C(5)	121(1)
C(4)	C(5)	C(6)	118(1)
C(1)	C(6)	C(5)	125(1)
N(8)	C(7)	C(1)	130(1)
C(12)	C(11)	C(16)	117(1)
C(12)	C(11)	C(17)	125(1)
C(16)	C(11)	C(17)	119(1)
O(20)	C(12)	C(11)	119(1)
O(20)	C(12)	C(13)	121(1)
C(11)	C(12)	C(13)	120(1)
C(12)	C(13)	C(14)	121(1)
C(13)	C(14)	C(15)	120(2)
C(14)	C(15)	C(16)	118(1)
C(11)	C(16)	C(15)	123(1)
N(18)	C(17)	C(11)	127(1)

Table S(6) Fractional atomic coordinates for [C₂₇H₃₃N₃O₇Sn₃]

Atom	x	y	z	B(eq) ^a
Sn(1)	-0.04434(4)	-0.11166(2)	0.64937(3)	3.655(9)
Sn(2)	0.12638(4)	-0.18294(2)	0.49754(3)	4.056(10)
Sn(3)	0.31021(4)	-0.18861(2)	0.70226(3)	4.36(1)
O(9)	-0.3568(4)	-0.0370(2)	0.5997(3)	6.1(1)
O(10)	-0.0772(4)	-0.1414(2)	0.4820(2)	4.41(10)
O(19)	0.1945(4)	-0.1736(2)	0.7946(2)	4.6(1)
O(20)	-0.1536(4)	-0.0587(2)	0.7311(2)	4.5(1)
O(30)	0.1259(4)	-0.1689(2)	0.6197(2)	4.03(9)
O(40)	0.3466(4)	-0.2096(2)	0.5734(3)	5.7(1)
O(50)	0.4225(5)	-0.3884(2)	0.5298(3)	7.0(1)
N(8)	-0.2766(5)	-0.0686(2)	0.5506(3)	4.6(1)
N(18)	0.1050(5)	-0.1216(2)	0.7797(3)	4.0(1)
N(38)	0.4041(5)	-0.2664(3)	0.5522(3)	5.3(1)
C(1)	-0.2895(6)	-0.0935(3)	0.4017(4)	4.2(1)
C(2)	-0.1656(7)	-0.1284(3)	0.4066(4)	4.4(2)
C(3)	-0.1361(7)	-0.1502(3)	0.3307(4)	5.9(2)
C(4)	-0.2218(9)	-0.1355(4)	0.2532(4)	6.5(2)
C(5)	-0.3435(9)	-0.1010(4)	0.2482(5)	6.9(2)
C(6)	-0.3750(7)	-0.0798(3)	0.3217(4)	5.3(2)
C(7)	-0.3381(6)	-0.0671(3)	0.4721(4)	4.7(2)
C(11)	0.0361(7)	-0.0261(3)	0.8424(4)	4.6(2)
C(12)	-0.0943(7)	-0.0162(3)	0.7884(4)	4.4(2)
C(13)	-0.1663(8)	0.0396(3)	0.7979(4)	5.8(2)
C(14)	-0.1117(10)	0.0828(4)	0.8597(5)	7.4(2)
C(15)	0.017(1)	0.0719(4)	0.9154(5)	7.9(3)
C(16)	0.0890(8)	0.0180(3)	0.9075(4)	6.3(2)
C(17)	0.1219(6)	-0.0828(3)	0.8418(4)	4.3(1)
C(21)	-0.1678(7)	-0.1928(3)	0.6555(4)	5.5(2)
C(22)	0.0485(6)	-0.0287(3)	0.6155(4)	4.3(1)
C(23)	0.2242(7)	-0.1133(3)	0.4362(4)	6.2(2)
C(24)	0.0683(7)	-0.2760(3)	0.4610(4)	5.8(2)
C(25)	0.4290(7)	-0.1042(4)	0.7117(4)	6.7(2)
C(26)	0.3670(8)	-0.2793(4)	0.7509(5)	7.4(2)
C(31)	0.5563(6)	-0.3111(3)	0.4724(4)	4.6(2)
C(32)	0.5185(7)	-0.3733(4)	0.4843(4)	5.2(2)

C(33)	0.5804(9)	-0.4226(4)	0.4495(5)	7.1(2)
C(34)	0.6778(9)	-0.4105(5)	0.4038(5)	7.6(3)
C(35)	0.7170(8)	-0.3506(5)	0.3897(5)	6.8(2)
C(36)	0.6572(7)	-0.3007(4)	0.4251(5)	6.7(2)
C(37)	0.4931(7)	-0.2584(3)	0.5057(4)	4.9(2)
H(3)	-0.0549	-0.1757	0.3330	7.0246
H(4)	-0.1969	-0.1492	0.2027	7.8478
H(5)	-0.4045	-0.0920	0.1948	8.2476
H(6)	-0.4576	-0.0549	0.3182	6.3062
H(7)	-0.4268	-0.0461	0.4583	5.6791
H(9)	-0.3233	-0.0344	0.6595	7.2932
H(13)	-0.2552	0.0477	0.7606	7.0004
H(14)	-0.1625	0.1205	0.8643	8.9034
H(15)	0.0546	0.1016	0.9586	9.4998
H(16)	0.1764	0.0099	0.9464	7.5114
H(17)	0.1948	-0.0913	0.8906	5.2070
H(21a)	-0.2548	-0.1807	0.6683	6.5971
H(21b)	-0.1861	-0.2140	0.6024	6.5971
H(21c)	-0.1181	-0.2202	0.6985	6.5971
H(22a)	0.1406	-0.0239	0.6508	5.1580
H(22b)	0.0548	-0.0313	0.5580	5.1580
H(22c)	-0.0079	0.0067	0.6227	5.1580
H(23a)	0.2744	-0.0845	0.4772	7.4526
H(23b)	0.2880	-0.1330	0.4077	7.4526
H(23c)	0.1539	-0.0912	0.3962	7.4526
H(24a)	0.0145	-0.2931	0.4978	7.0056
H(24b)	0.0132	-0.2762	0.4044	7.0056
H(24c)	0.1509	-0.3007	0.4642	7.0056
H(25a)	0.5231	-0.1137	0.7084	8.0170
H(25b)	0.3873	-0.0767	0.6666	8.0170
H(25c)	0.4299	-0.0843	0.7644	8.0170
H(26a)	0.2841	-0.3039	0.7476	8.8622
H(26b)	0.4255	-0.2990	0.7187	8.8622
H(26c)	0.4171	-0.2761	0.8085	8.8622
H(33)	0.5543	-0.4649	0.4578	8.5120
H(34)	0.7200	-0.4448	0.3810	9.1331
H(35)	0.7840	-0.3430	0.3562	8.1209
H(36)	0.6858	-0.2587	0.4169	8.0054

H(37)	0.5178	-0.2167	0.4929	5.8990
H(50)	0.3777	-0.3560	0.5546	8.4199

$$a B_{eq} = (8\pi^2/3)(\underline{U}_{11}(aa^*)^2 + \underline{U}_{22}(bb^*)^2 + \underline{U}_{33}(cc^*)^2 + 2\underline{U}_{12}aa^*bb^*\cos\gamma + 2\underline{U}_{13}aa^*cc^*\cos\beta + 2\underline{U}_{23}bb^*cc^*\cos\alpha)$$

Table S(7) **Anisotropic thermal parameters ($\text{\AA}^2$) for $[\text{C}_{27}\text{H}_{33}\text{N}_3\text{O}_7\text{Sn}_3]$**

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn(1)	0.0444(2)	0.0461(2)	0.0497(2)	0.0005(2)	0.0134(2)	0.0027(2)
Sn(2)	0.0573(3)	0.0506(2)	0.0473(2)	0.0077(2)	0.0142(2)	0.0002(2)
Sn(3)	0.0535(3)	0.0561(3)	0.0531(2)	0.0120(2)	0.0061(2)	0.0002(2)
O(9)	0.058(3)	0.104(4)	0.072(3)	0.021(3)	0.022(2)	-0.002(3)
O(10)	0.050(2)	0.071(3)	0.043(2)	0.008(2)	0.005(2)	0.003(2)
O(19)	0.069(3)	0.057(3)	0.049(2)	0.022(2)	0.011(2)	0.010(2)
O(20)	0.052(2)	0.066(3)	0.056(3)	0.006(2)	0.018(2)	-0.006(2)
O(30)	0.052(2)	0.051(2)	0.050(2)	0.011(2)	0.012(2)	0.000(2)
O(40)	0.064(3)	0.085(3)	0.066(3)	0.027(3)	0.015(2)	-0.008(2)
O(50)	0.103(4)	0.083(4)	0.089(4)	0.010(3)	0.040(3)	0.008(3)
N(8)	0.044(3)	0.063(3)	0.070(4)	0.002(3)	0.016(3)	-0.002(3)
N(18)	0.054(3)	0.057(3)	0.044(3)	0.006(2)	0.015(2)	0.003(2)
N(38)	0.057(3)	0.076(4)	0.068(3)	0.016(3)	0.016(3)	-0.004(3)
C(1)	0.041(3)	0.052(4)	0.060(4)	-0.008(3)	0.002(3)	0.004(3)
C(2)	0.062(4)	0.049(4)	0.053(4)	-0.005(3)	0.009(3)	0.001(3)
C(3)	0.083(5)	0.071(5)	0.063(5)	0.021(4)	0.007(4)	-0.005(4)
C(4)	0.109(6)	0.083(5)	0.050(4)	-0.001(5)	0.004(4)	-0.002(4)
C(5)	0.086(6)	0.088(6)	0.069(5)	-0.005(5)	-0.020(4)	0.004(4)
C(6)	0.051(4)	0.064(4)	0.074(5)	-0.003(3)	-0.009(4)	0.013(4)
C(7)	0.043(4)	0.066(4)	0.066(4)	-0.003(3)	0.003(3)	0.004(4)
C(11)	0.077(5)	0.058(4)	0.045(3)	0.002(4)	0.020(3)	0.001(3)
C(12)	0.067(4)	0.055(4)	0.051(4)	0.006(3)	0.027(3)	0.005(3)
C(13)	0.082(5)	0.077(5)	0.063(4)	0.023(4)	0.019(4)	0.004(4)
C(14)	0.123(7)	0.072(5)	0.083(6)	0.034(5)	0.015(5)	-0.011(5)
C(15)	0.137(8)	0.080(6)	0.075(5)	0.017(6)	0.008(5)	-0.030(5)
C(16)	0.099(6)	0.072(5)	0.061(4)	0.011(4)	0.006(4)	-0.012(4)
C(17)	0.063(4)	0.058(4)	0.043(3)	-0.001(3)	0.009(3)	0.003(3)
C(21)	0.072(5)	0.064(4)	0.074(4)	-0.019(4)	0.018(4)	0.000(4)
C(22)	0.051(4)	0.051(4)	0.061(4)	0.002(3)	0.012(3)	0.009(3)
C(23)	0.078(5)	0.078(5)	0.088(5)	0.007(4)	0.037(4)	0.014(4)
C(24)	0.089(5)	0.058(4)	0.075(5)	0.003(4)	0.019(4)	-0.009(4)
C(25)	0.071(5)	0.093(6)	0.084(5)	-0.020(4)	0.007(4)	-0.014(4)
C(26)	0.116(7)	0.080(6)	0.077(5)	0.029(5)	0.007(5)	0.009(4)
C(31)	0.046(4)	0.078(5)	0.048(4)	0.010(3)	0.005(3)	-0.006(3)
C(32)	0.053(4)	0.090(5)	0.051(4)	0.019(4)	0.003(3)	-0.002(4)

C(33)	0.090(6)	0.096(6)	0.082(5)	0.028(5)	0.017(5)	-0.001(5)
C(34)	0.076(6)	0.121(8)	0.092(6)	0.031(6)	0.018(5)	-0.019(6)
C(35)	0.061(5)	0.129(8)	0.073(5)	-0.001(5)	0.026(4)	-0.019(5)
C(36)	0.051(4)	0.115(7)	0.091(6)	-0.012(4)	0.024(4)	-0.024(5)
C(37)	0.050(4)	0.079(5)	0.055(4)	0.005(3)	0.007(3)	-0.007(3)

where the anisotropic thermal parameter is given by the expression:

$$T_{\text{aniso}} = \exp[-2\pi^2(h^2a^2U_{11} + k^2b^2U_{22} + l^2c^2U_{33} + 2hka*b*U_{12} + 2hla*c*U_{13} + 2klb*c*U_{23})].$$

Table S(8) **All bond distances (Å) for [C₂₇H₃₃N₃O₇Sn₃]**

atom	atom	distance	atom	atom	distance
Sn(1)	O(10)	2.729(4)	N(18)	C(17)	1.281(7)
Sn(1)	O(20)	2.186(4)	N(38)	C(37)	1.281(7)
Sn(1)	O(30)	2.191(4)	C(1)	C(2)	1.400(8)
Sn(1)	N(8)	2.614(5)	C(1)	C(6)	1.401(8)
Sn(1)	N(18)	2.282(5)	C(1)	C(7)	1.442(8)
Sn(1)	C(21)	2.111(6)	C(2)	C(3)	1.401(8)
Sn(1)	C(22)	2.106(6)	C(3)	C(4)	1.375(9)
Sn(2)	O(10)	2.127(4)	C(4)	C(5)	1.38(1)
Sn(2)	O(30)	2.001(4)	C(5)	C(6)	1.370(9)
Sn(2)	O(40)	2.282(5)	C(11)	C(12)	1.382(8)
Sn(2)	C(23)	2.120(7)	C(11)	C(16)	1.415(8)
Sn(2)	C(24)	2.098(6)	C(11)	C(17)	1.463(8)
Sn(3)	O(19)	2.089(4)	C(12)	C(13)	1.400(8)
Sn(3)	O(30)	2.019(4)	C(13)	C(14)	1.37(1)
Sn(3)	O(40)	2.239(4)	C(14)	C(15)	1.38(1)
Sn(3)	C(25)	2.115(7)	C(15)	C(16)	1.360(9)
Sn(3)	C(26)	2.103(7)	C(31)	C(32)	1.394(9)
O(9)	N(8)	1.404(6)	C(31)	C(36)	1.392(8)
O(10)	C(2)	1.352(7)	C(31)	C(37)	1.437(8)
O(19)	N(18)	1.390(5)	C(32)	C(33)	1.388(9)
O(20)	C(12)	1.327(7)	C(33)	C(34)	1.35(1)
O(40)	N(38)	1.402(6)	C(34)	C(35)	1.36(1)
O(50)	C(32)	1.352(7)	C(35)	C(36)	1.39(1)
N(8)	C(7)	1.276(7)			

Table S(9) **All bond angles (°) for [C₂₇H₃₃N₃O₇Sn₃]**

atom	atom	atom	angle	atom	atom	atom	angle
O(10)	Sn(1)	O(20)	139.2(1)	O(30)	Sn(2)	C(23)	117.5(2)
O(10)	Sn(1)	O(30)	65.0(1)	O(30)	Sn(2)	C(24)	110.9(2)
O(10)	Sn(1)	N(8)	65.4(1)	O(40)	Sn(2)	C(23)	87.7(2)
O(10)	Sn(1)	N(18)	143.4(1)	O(40)	Sn(2)	C(24)	94.5(2)
O(10)	Sn(1)	C(21)	85.4(2)	C(23)	Sn(2)	C(24)	129.9(3)
O(10)	Sn(1)	C(22)	83.9(2)	O(19)	Sn(3)	O(30)	84.4(2)
O(20)	Sn(1)	O(30)	155.8(1)	O(19)	Sn(3)	O(40)	157.2(2)
O(20)	Sn(1)	N(8)	73.8(2)	O(19)	Sn(3)	C(25)	101.1(2)
O(20)	Sn(1)	N(18)	77.3(2)	O(19)	Sn(3)	C(26)	90.5(2)
O(20)	Sn(1)	C(21)	91.7(2)	O(30)	Sn(3)	O(40)	74.2(1)
O(20)	Sn(1)	C(22)	91.4(2)	O(30)	Sn(3)	C(25)	105.1(2)
O(30)	Sn(1)	N(8)	130.4(2)	O(30)	Sn(3)	C(26)	123.7(2)
O(30)	Sn(1)	N(18)	78.4(2)	O(40)	Sn(3)	C(25)	92.1(2)
O(30)	Sn(1)	C(21)	91.4(2)	O(40)	Sn(3)	C(26)	94.8(2)
O(30)	Sn(1)	C(22)	90.9(2)	C(25)	Sn(3)	C(26)	130.8(3)
N(8)	Sn(1)	N(18)	151.2(2)	Sn(1)	O(10)	Sn(2)	94.8(1)
N(8)	Sn(1)	C(21)	83.8(2)	Sn(1)	O(10)	C(2)	139.2(3)
N(8)	Sn(1)	C(22)	84.9(2)	Sn(2)	O(10)	C(2)	124.9(3)
N(18)	Sn(1)	C(21)	97.4(2)	Sn(3)	O(19)	N(18)	114.5(3)
N(18)	Sn(1)	C(22)	95.6(2)	Sn(1)	O(20)	C(12)	125.4(4)
C(21)	Sn(1)	C(22)	166.9(2)	Sn(1)	O(30)	Sn(2)	118.1(2)
O(10)	Sn(2)	O(30)	81.0(1)	Sn(1)	O(30)	Sn(3)	124.7(2)
O(10)	Sn(2)	O(40)	154.0(1)	Sn(2)	O(30)	Sn(3)	115.0(2)
O(10)	Sn(2)	C(23)	99.2(2)	Sn(2)	O(40)	Sn(3)	97.2(2)
O(10)	Sn(2)	C(24)	99.9(2)	Sn(2)	O(40)	N(38)	117.2(3)
O(30)	Sn(2)	O(40)	73.6(1)	Sn(3)	O(40)	N(38)	123.7(3)
Sn(1)	N(8)	O(9)	109.4(3)	C(14)	C(15)	C(16)	119.1(7)
Sn(1)	N(8)	C(7)	139.5(4)	C(11)	C(16)	C(15)	121.2(7)
O(9)	N(8)	C(7)	111.0(5)	N(18)	C(17)	C(11)	124.1(6)
Sn(1)	N(18)	O(19)	118.3(3)	C(32)	C(31)	C(36)	117.9(6)
Sn(1)	N(18)	C(17)	127.5(4)	C(32)	C(31)	C(37)	122.2(6)
O(19)	N(18)	C(17)	114.2(5)	C(36)	C(31)	C(37)	119.9(7)
O(40)	N(38)	C(37)	113.0(5)	O(50)	C(32)	C(31)	122.4(6)
C(2)	C(1)	C(6)	118.8(6)	O(50)	C(32)	C(33)	117.4(7)

C(2)	C(1)	C(7)	126.3(6)	C(31)	C(32)	C(33)	120.2(7)
C(6)	C(1)	C(7)	114.8(6)	C(32)	C(33)	C(34)	120.1(8)
O(10)	C(2)	C(1)	121.3(5)	C(33)	C(34)	C(35)	121.8(8)
O(10)	C(2)	C(3)	120.7(6)	C(34)	C(35)	C(36)	118.7(7)
C(1)	C(2)	C(3)	118.0(6)	C(31)	C(36)	C(35)	121.2(8)
C(2)	C(3)	C(4)	121.6(7)	N(38)	C(37)	C(31)	121.4(6)
C(3)	C(4)	C(5)	120.5(7)				
C(4)	C(5)	C(6)	118.8(7)				
C(1)	C(6)	C(5)	122.2(6)				
N(8)	C(7)	C(1)	127.9(6)				
C(12)	C(11)	C(16)	119.7(6)				
C(12)	C(11)	C(17)	124.2(6)				
C(16)	C(11)	C(17)	115.9(6)				
O(20)	C(12)	C(11)	121.9(6)				
O(20)	C(12)	C(13)	120.2(6)				
C(11)	C(12)	C(13)	117.9(6)				
C(12)	C(13)	C(14)	121.6(7)				
C(13)	C(14)	C(15)	120.4(7)				