Supplementary Information

Evaluation of Sn(II) Aminoalkoxide Precursors for Atomic Layer Deposition of SnO Thin Films.

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Table 1S: Crystal and structure refinement data for 1a-d and 2a-d.

Compound reference	**1a**	**1b**	**1c**	**1d**	**2a**	**2b**	**2c**	**2d**
Chemical formula	$C_{12}H_{32}N_4O_2Sn_2$	$C_{14}H_{36}N_4O_2Sn_2$	$C_{16}H_{40}N_4O_2Sn_2$	$C_{16}H_{28}F_{12}N_4O_2Sn_2$	$C_{20}H_{56}N_4O_2Si_4Sn_2$	$C_{22}H_{60}N_4O_2Si_4Sn_2$	$C_{24}H_{64}N_4O_2Si_4Sn_2$	$C_{12}H_{26}F_6N_2OSi_2Sn$
Formula Mass	501.79	529.85	557.90	773.80	734.42	762.48	790.53	503.22
Crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic	Triclinic	Orthorhombic	Monoclinic	Triclinic
a/Å	6.78330(10)	7.5712(4)	9.2945(3)	12.5872(3)	8.7579(4)	20.53720(10)	8.6975(5)	7.06130(10)
b/Å	17.20280(10)	8.6744(5)	11.9266(4)	8.5519(2)	8.9319(4)	12.18560(10)	14.292(3)	8.48480(10)
c/Å	8.14230(10)	9.2638(4)	10.7094(4)	12.5367(3)	23.8923(19)	14.37850(10)	15.194(3)	18.7724(2)
α/°	90	73.154(5)	90	90	80.516(5)	90	90	94.6970(10)
β/°	95.9880(10)	74.104(5)	100.737(4)	100.094(3)	86.651(5)	90	93.032(11)	98.7470(10)
γ/°	90	68.138(5)	90	90	68.460(4)	90	90	110.7630(10)
Unit cell volume/Å^3	944.955(19)	530.90(5)	1166.37(7)	1328.62(6)	1714.68(18)	3598.34(4)	1886.0(5)	1028.16(2)
Temperature/K	150(2)	150(2)	150(2)	150(2)	150(2)	150(2)	150(2)	150(2)
Space group	$P2_1/n$	*P***Error!**	$P2_1/n$	$P2_1/c$	*P***Error!**	$Pca2_1$	$P2_1/n$	*P***Error!**
No. of formula units per unit cell, *Z*	2	1	2	2	2	4	2	2
Radiation type	Cu Kα	Cu Kα	Mo Kα	Cu Kα	Mo Kα	Cu Kα	Mo Kα	Cu Kα
Absorption coefficient, μ/mm^{-1}	21.080	18.795	2.156	15.946	1.618	12.523	1.476	11.530
No. of reflections measured	18198	3776	7109	9233	7177	35425	21534	34240
No. of independent reflections	1884	2104	2261	2647	7177	6731	4216	4091
R_{int}	0.0404	0.0224	0.0542	-	-	0.0390	0.0347	0.0419
Final R_1 values ($I > 2\sigma(I)$)	0.0173	0.0297	0.0339	0.0425	0.0443	0.0426	0.0238	0.0323
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.0431	0.0792	0.0538	0.1362	0.1049	0.1115	0.0456	0.0845
Final R_1 values (all data)	0.0183	0.0304	0.0462	0.0567	0.0461	0.0430	0.0288	0.0323
Final $wR(F^2)$ values (all data)	0.0437	0.0799	0.0606	0.1385	0.1072	0.1119	0.0473	0.0845
Goodness of fit on F^2	1.048	1.103	1.036	1.095	1.085	1.065	1.067	1.153
Flack parameter	-	-	-	-	-	0.34(12)	-	-
CSD Number	2055540	2055535	2055536	2055538	2055542	2055545	2055534	2055544

Table 2S: Crystal and structure refinement data for 3a-d.

Compound reference	**3a**	**3b**	**3c**	**3d**
Chemical formula	$C_8H_{20}N_2O_2Sn$	$C_{10}H_{24}N_2O_2Sn$	$C_{12}H_{28}N_2O_2Sn$	$C_{12}H_{16}F_{12}N_2O_2Sn$
Formula Mass	294.95	323.00	351.05	566.96
Crystal system	Orthorhombic	Monoclinic	Orthorhombic	Monoclinic
a/Å	11.8081(2)	11.7352(4)	8.1592(3)	18.5031(2)
b/Å	10.1306(2)	10.3182(3)	13.8664(5)	8.29960(10)
c/Å	10.0735(2)	12.0111(4)	14.1626(5)	12.5214(2)
α/°	90	90	90	90
β/°	90	95.166(3)	90	94.4840(10)
γ/°	90	90	90	90
Unit cell volume/Å^3	1205.02(4)	1448.47(8)	1602.34(10)	1917.00(4)
Temperature/K	150(2)	150(2)	150(2)	150(2)
Space group	Aba_2	$C2/c$	$P2_12_12_1$	$P2_1/c$
No. of formula units per unit cell, *Z*	4	4	4	4
Radiation type	Mo Kα	Mo Kα	Mo Kα	Cu Kα
Absorption coefficient, *μ*/mm^{-1}	2.097	1.752	1.590	11.814
No. of reflections measured	32894	6274	13388	13270
No. of independent reflections	1410	1660	3800	3815
R_{int}	0.0673	0.0303	0.0348	0.0343
Final R_1 values ($I > 2\sigma(I)$)	0.0255	0.0195	0.0252	0.0339
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.0509	0.0418	0.0422	0.0894
Final R_1 values (all data)	0.0287	0.0212	0.0283	0.0353
Final $wR(F^2)$ values (all data)	0.0521	0.0424	0.0430	0.0909
Goodness of fit on F^2	1.211	1.072	1.051	1.044
Flack parameter	0.47(8)	-	0.16(3)	-
CSD Number	2055537	2055541	2055543	2055539

Additional Crystallographic Details

1d: The data pertaining to the structure of **1d** were integrated to take account of twinning. The twin fractions are in a 13:87 ratio and, while the final residuals are not as low as one might wish, the structural assignments is unambiguous. The diffraction maxima became very smeared at higher Bragg angles for this sample.

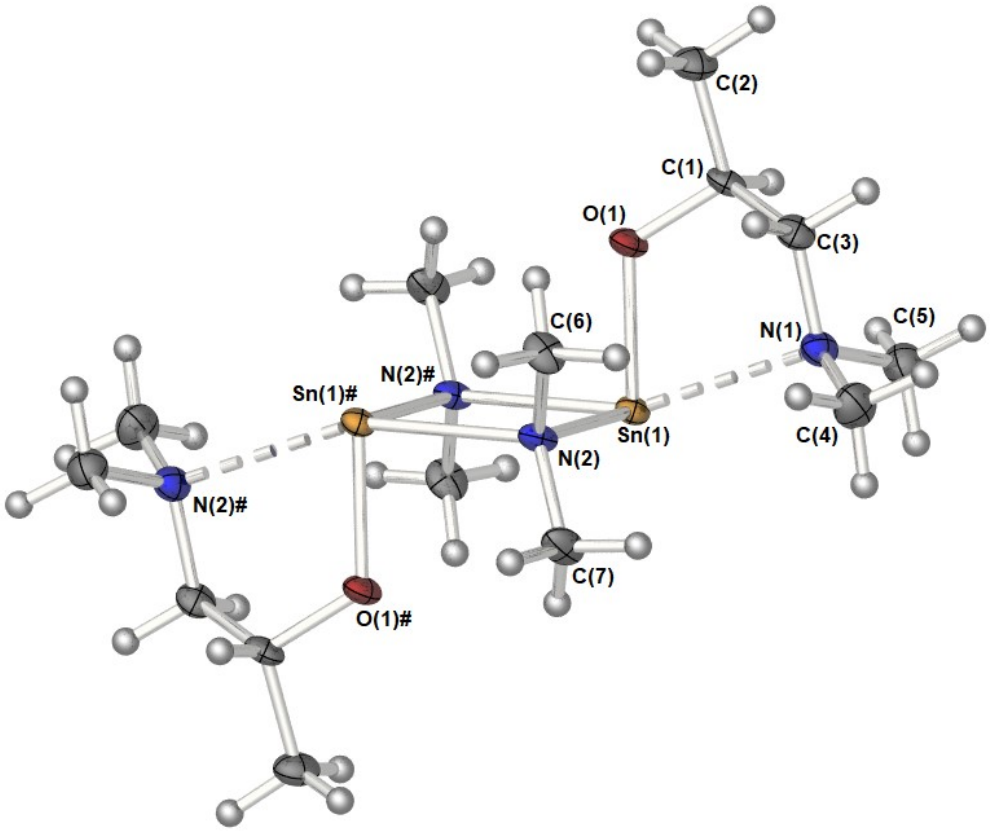

Figure S1: Molecular structure of $[(Me_2NCH_2C(H)MeO)Sn(\mu\text{-}NMe_2)]_2$ (1b). Thermal ellipsoids are shown at 50% probability. Symmetry transformations used to generate equivalent atoms: 1-X, 1-Y,1-Z.

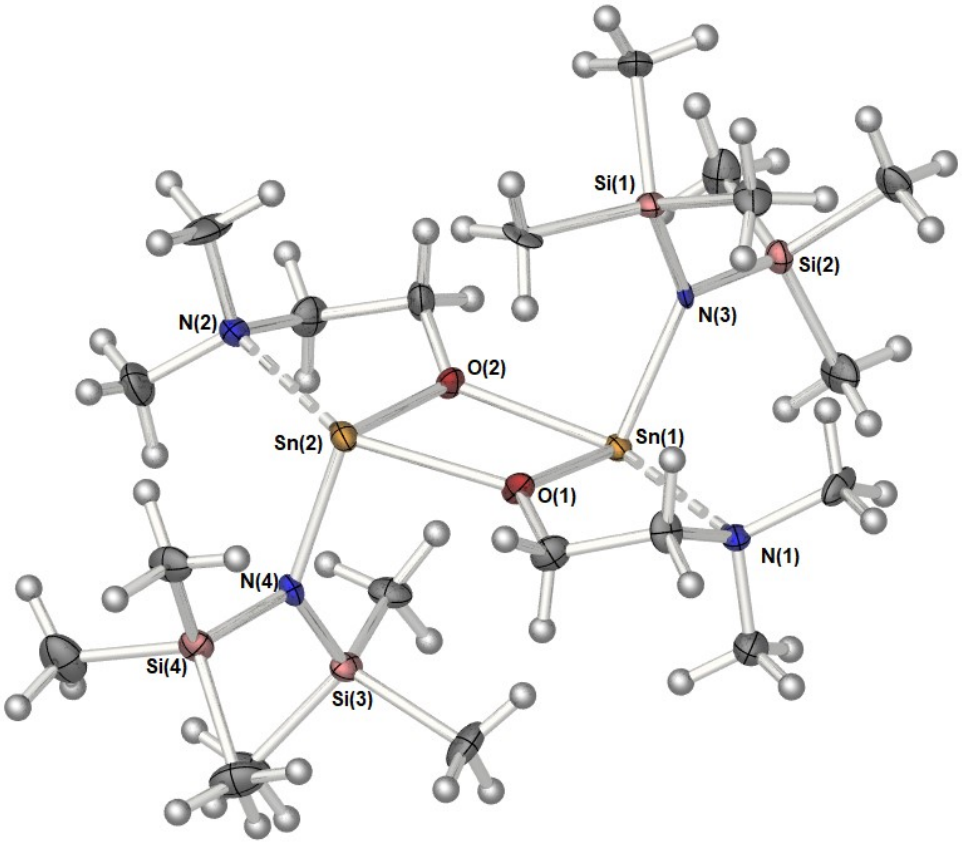

Figure S2: Molecular structure of $[\{(Me_3Si)_2N\}Sn(\mu\text{-}OCH_2CH_2Me_2)]_2$ (**2a**). Thermal ellipsoids are shown at 50% probability.

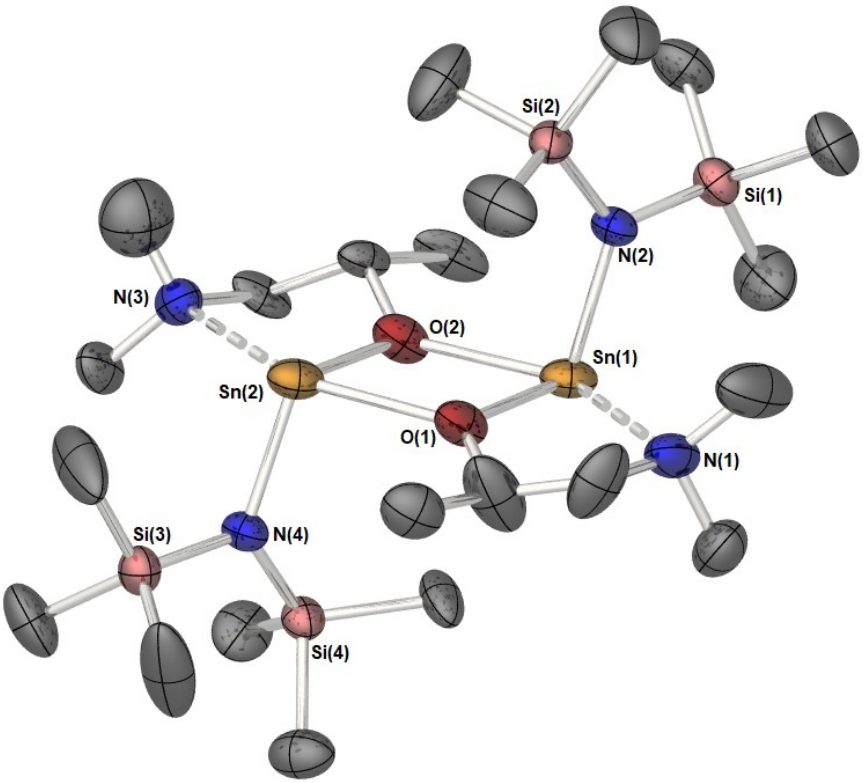

Figure S3: Molecular structure of [{$(Me_3Si)_2N$}Sn(μ-OC(H)MeCH_2Me_2)]$_2$ (2b). Thermal ellipsoids are shown at 50% probability. Hydrogen atoms have been omitted for clarity. Disorder in the ligand backbone [N(3), C(21)-C(25) and N(3A), C(21A)-C(25A)] and the HMDS ligand [C(15)-C(17) and C(15A)-C(17A)] have been omitted for clarity.

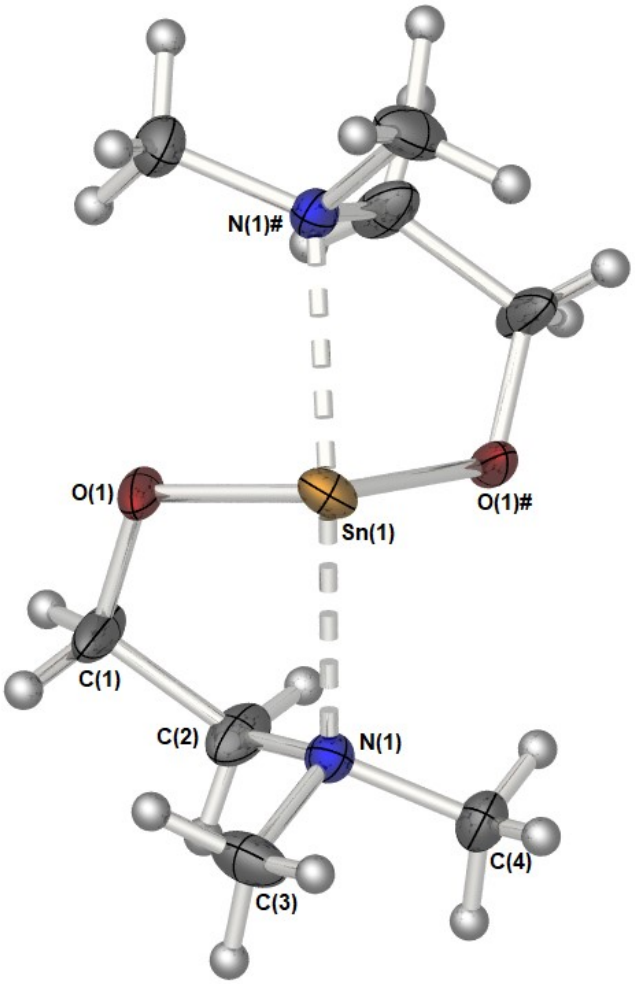

Figure S4: Molecular structure of [Sn($OCH_2CH_2Me_2$)$_2$] (3a). Thermal ellipsoids are shown at 50% probability. Symmetry transformations used to generate equivalent atoms: 1-X,1-Y, Z.

Table 3S – Evaporation rates of of [Sn{dmae}$_2$] (**3a**), [Sn{dmap}$_2$] (**3b**), [Sn{dmamp}$_2$] (**3c**) and [Sn{Fdmamp}$_2$] (**3d**) at 70°C.

Compound	Evaporation rate (μg min^{-1} cm^{-2})
3a	33.7
3b	55.0
3c	118.7
3d	36.8

References

[1] J. H. Han, Y. J. Chung, B. K. Park, S. K. Kim, H.-S. Kim, C. G. Kim, T.-M. Chung, *Chemistry of Materials* **2014**, *26*, 6088-6091.