Supporting Information

Volatile and Thermally Stable Polymeric Tin Trifluoroacetates

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Supplementary Figures and Tables

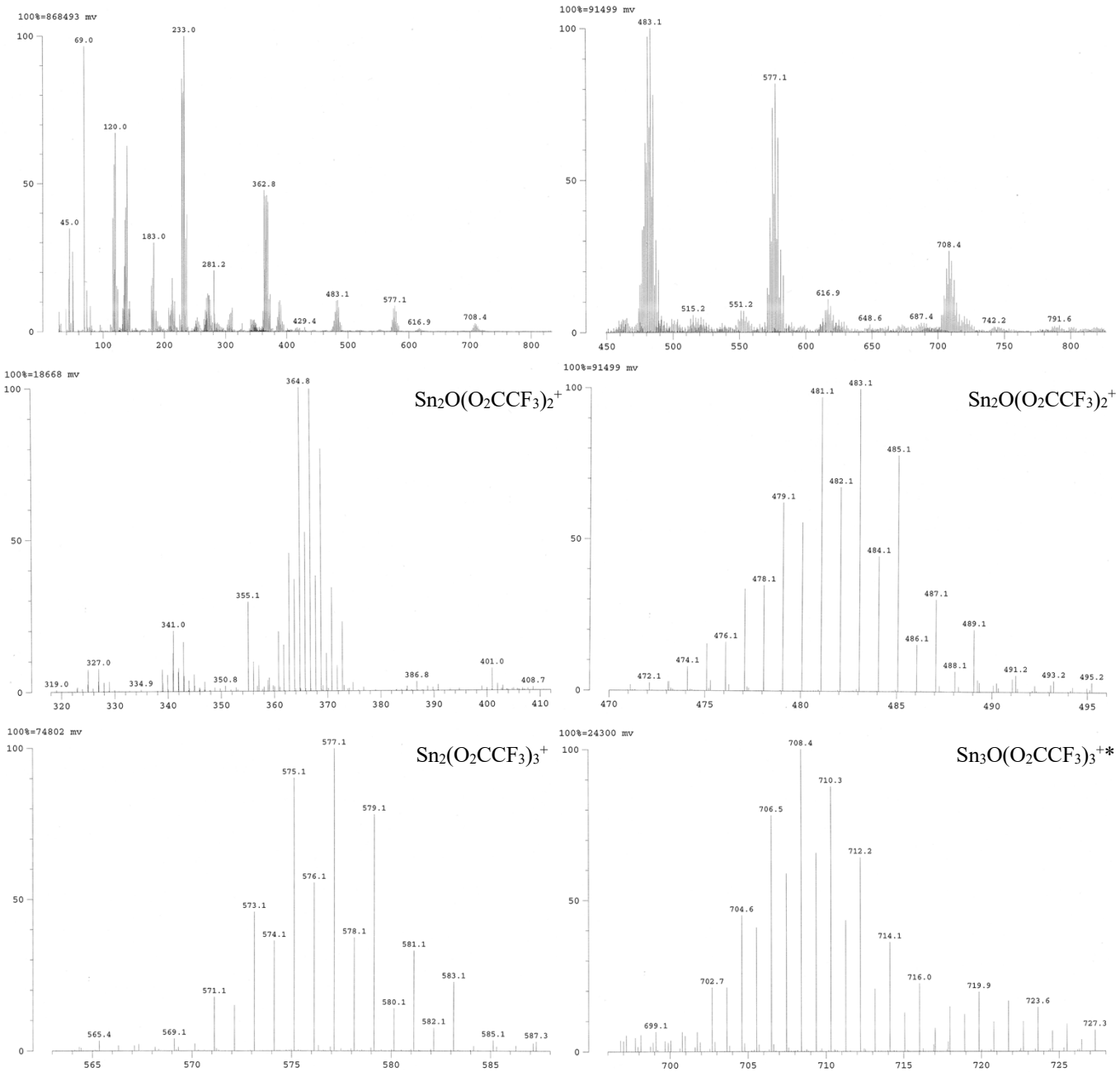

Figure S1. Electron-ionization mass spectrograms (EIMS) of **3**. Isotope patterns are labeled by their matching exact mass formulae. *Note:* the upper limit of accurate mass determination on this instrument was ~600 *m*/*z*, so the last ion ($Sn_3O(O_2CCF_3)_3^+$, bottom-right) could not be unambiguously identified. However, the isotope pattern clearly showed the presence of 3 Sn atoms in the ion, which supports our identification.

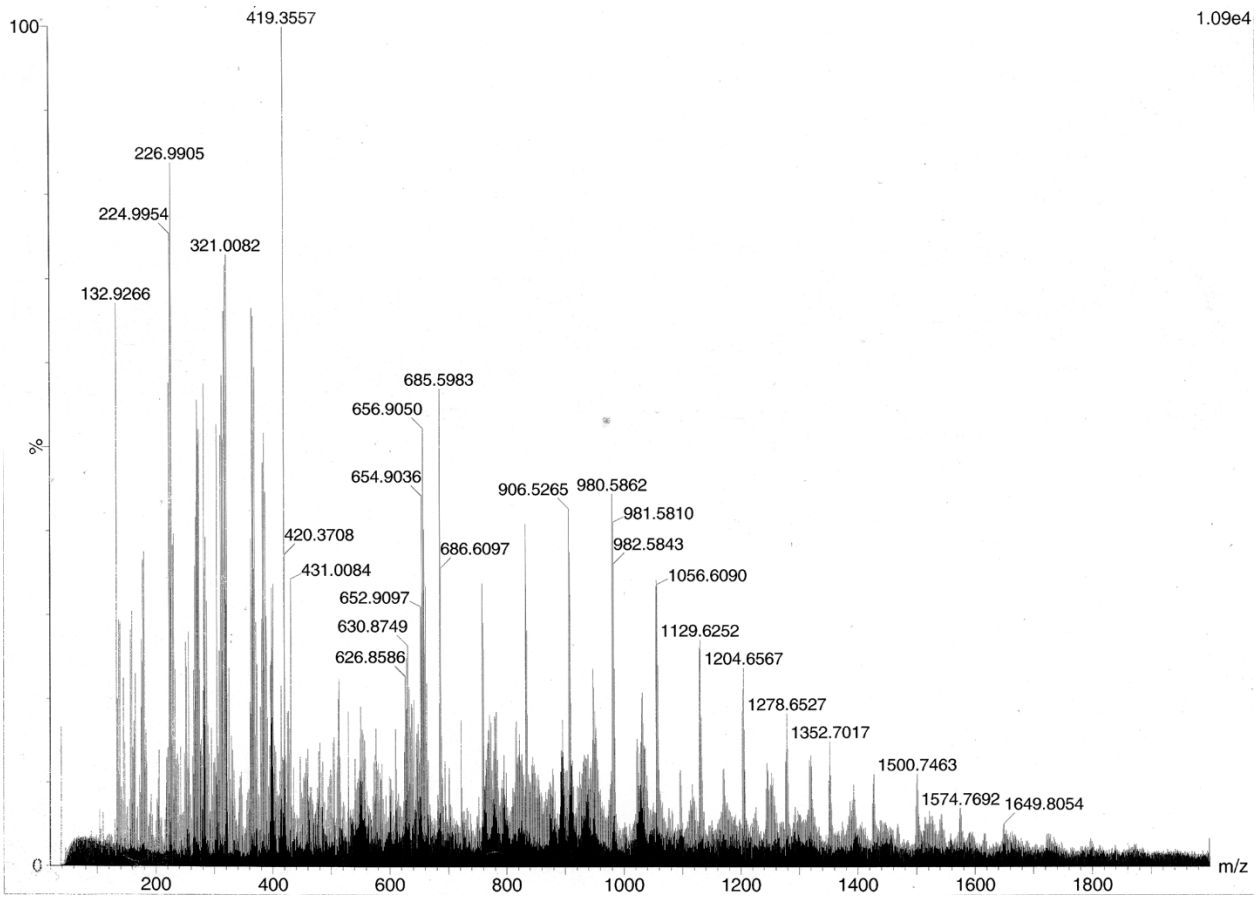

Figure S2. Electrospray ionization (ESI^+) mass spectrograms of **3** in acetonitrile.

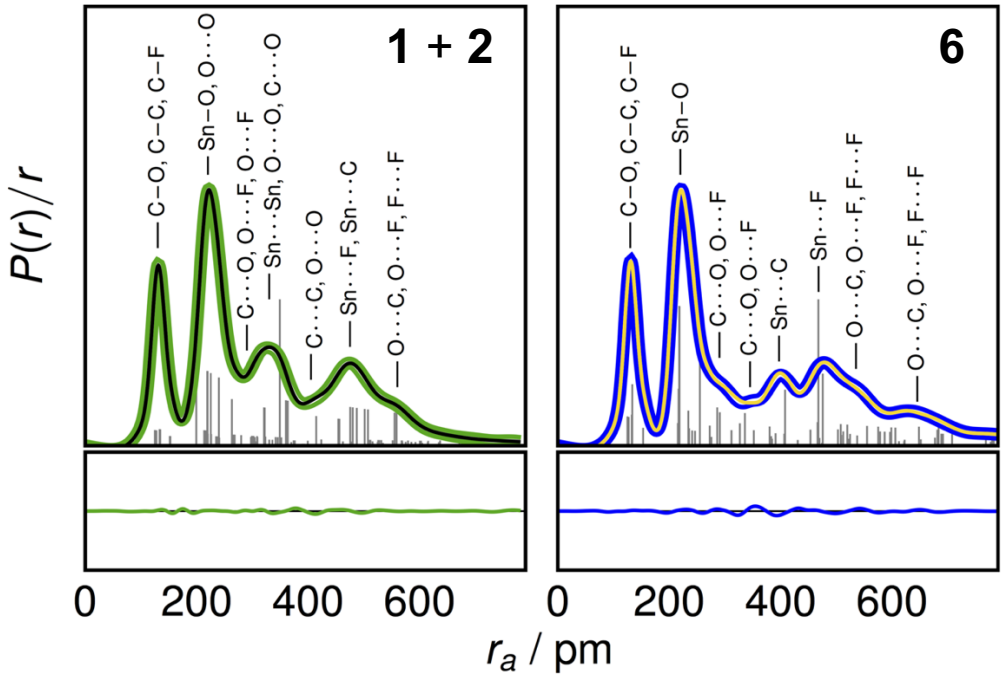

Figure S3: Radial distribution curve (RDC, top) and difference curve (bottom) for **3** (left) and **5** (right) collected by GED. Experimental data for **3** (right, black with green highlight) were compared to theoretically calculated RDCs for different molar ratios of **1** and **2** (white), and the best fit at 52:48 (95% confidence) was plotted here (R_G = 4.2% and R_D = 2.9%). Similarly, **5** (left, white with blue highlight) was compared to its DFT optimized structure (gold) and found to be monomeric **6** in the gas phase (R_G = 5.0% and R_D = 3.7%).

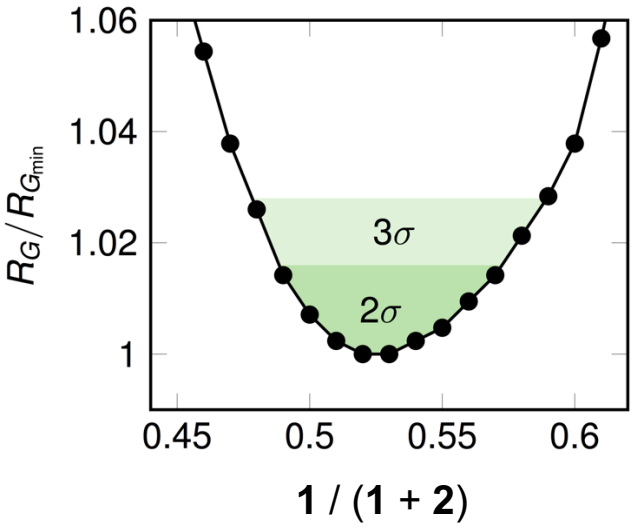

Figure S4: Quality of least-squares refinement $R_G/R_{G_{min}}$ of GED data of **3** as a function of the mole fraction of **1** and **2**. The well minimum is between 0.52-0.53, and 0.500 lies within 2σ of the minimum (i.e., 95% confidence). This confirmed bulk **3** thermally depolymerizes into an equimolar mixture of **1** and **2** upon evaporation.

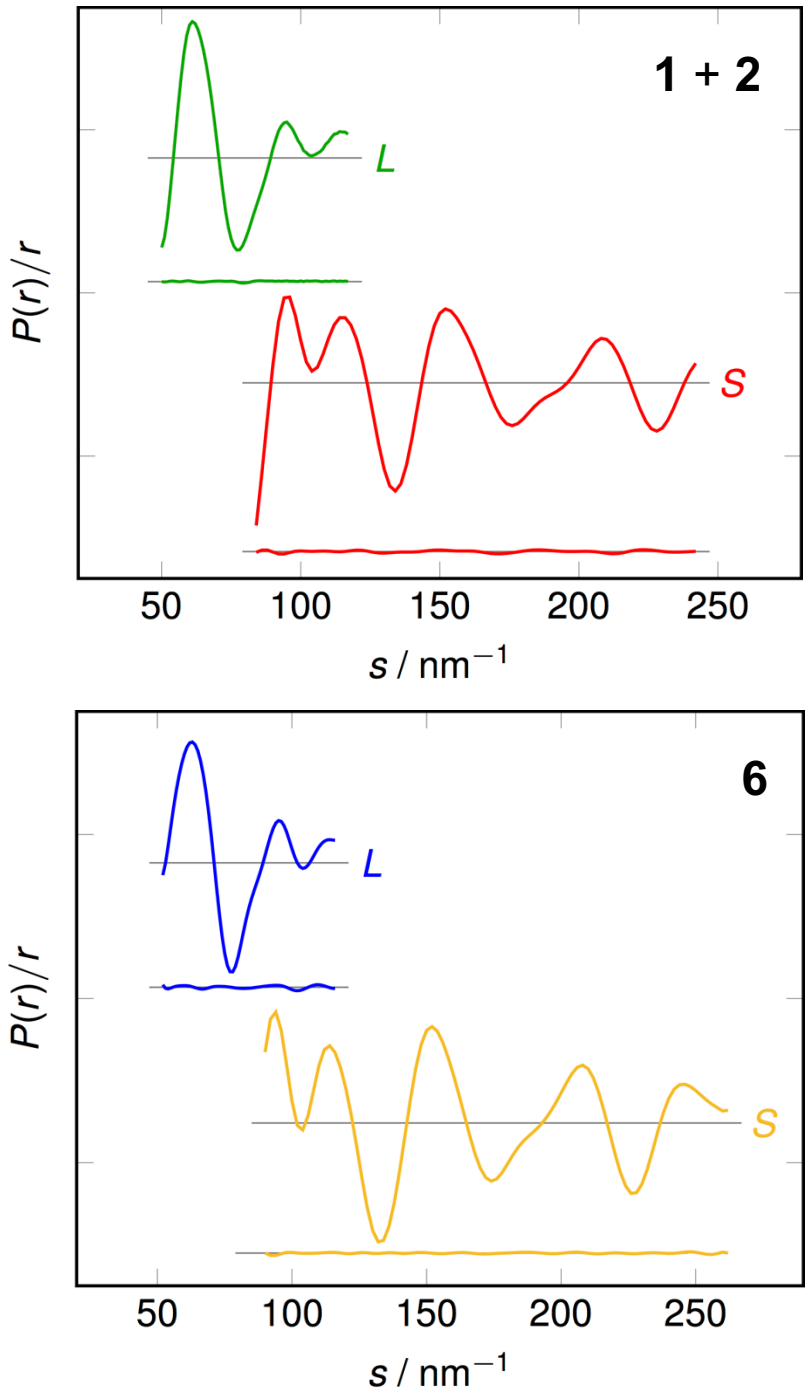

Figure S5. Molecular intensity curves for **1**+**2** (top) and **6** (bottom) obtained from gas phase electron diffraction at long (*L*) and short (*S*) nozzle distances. Difference curves for each are shown below.

Crystallography of hexatin(II) di-μ_3-oxy-octakis-μ-trifluoroacetate (3)

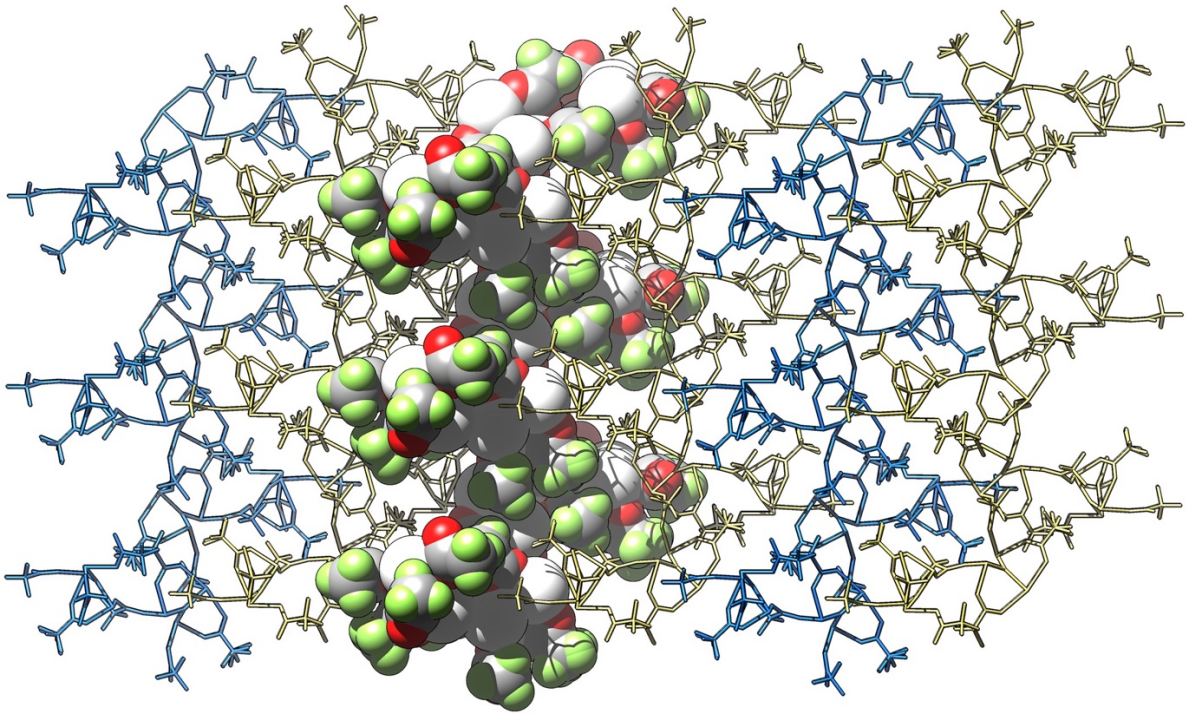

Figure S6. Crystal packing of a 3×3×3 supercell of **3**. Chains bound via Sn5–O18* bonds are depicted as single-colour stick diagrams (blue or gold), except for one that is displayed as a spacefilling diagram with the elements coloured as in the body text (e.g., Sn, white; O, red; F, green; C, grey). Fragments of chains surrounding the supercell have been omitted for clarity.

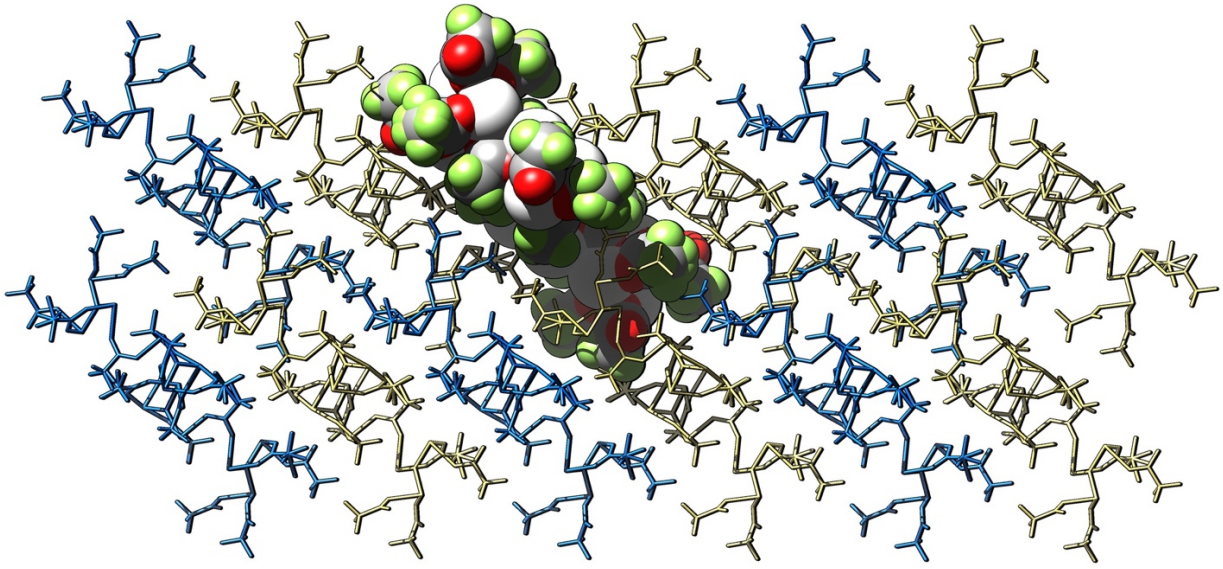

Figure S7. Crystal packing of a 3×3×3 supercell of **3**, viewed from the top of Figure S6.

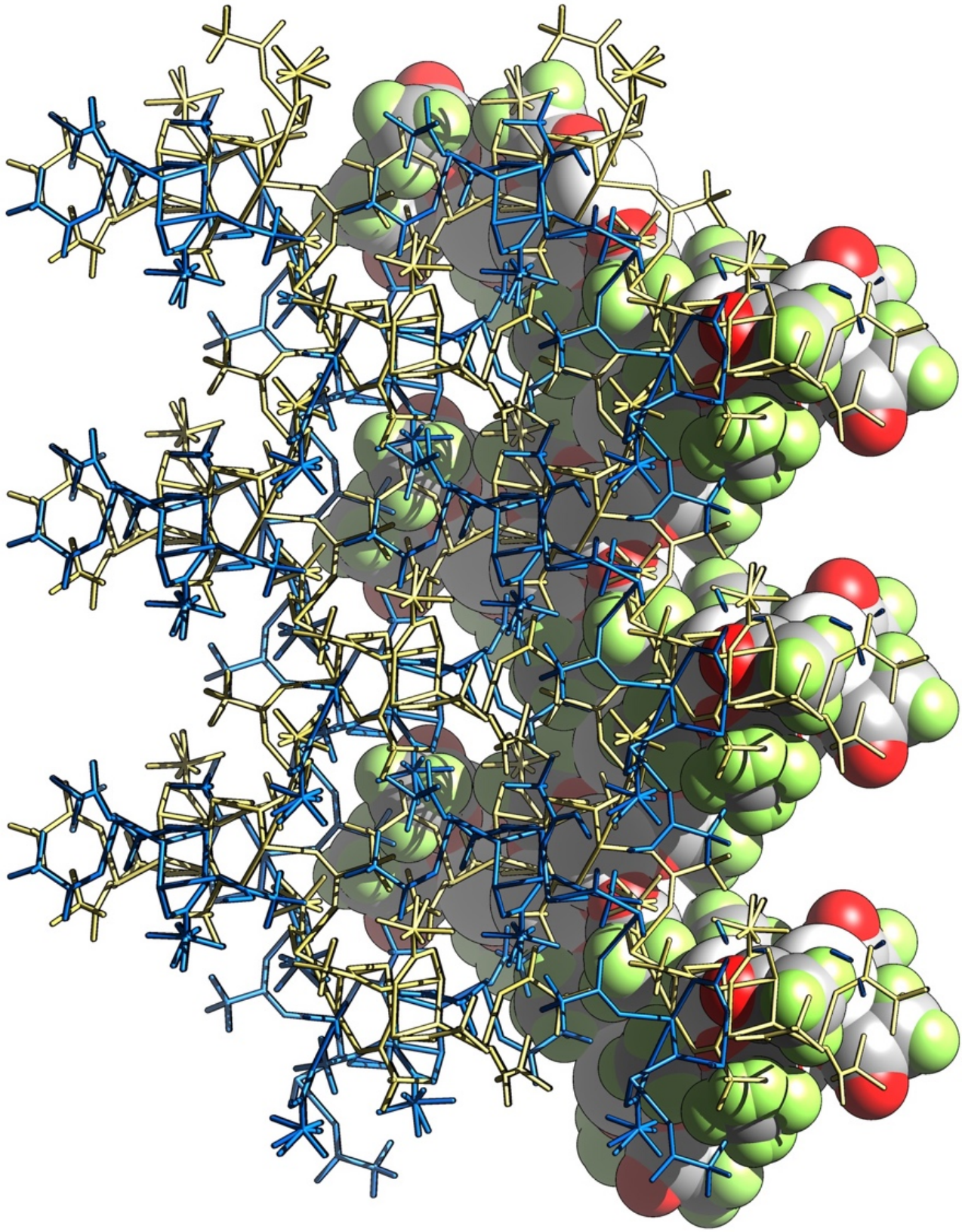

Figure S8. Crystal packing of a 3×3×3 supercell of **3**, viewed from the right of Figure S6.

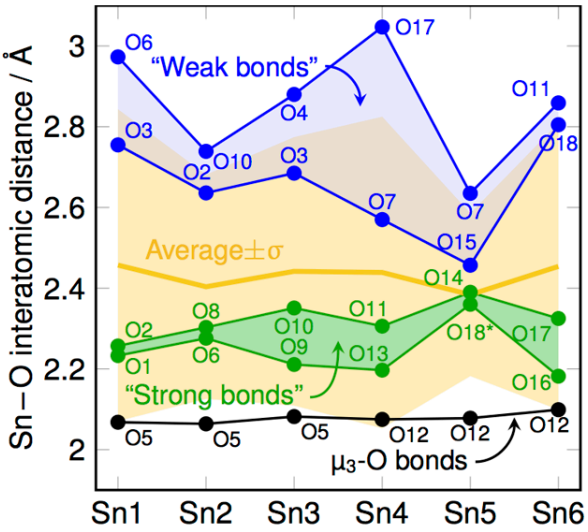

Figure S9. Bond definitions for **3**. Sn–O bonds were clearly grouped into three types by comparing the five shortest Sn-O distances: two "weak bonds" (i.e., coordinative C–O→Sn bonds, longer than average, blue), two "strong bonds" (i.e., covalent C–O–Sn bonds, shorter than average, green), and one μ_3-bridging oxy bond (black, shortest, d < 2.1 Å). The average with standard deviation of these bonds is drawn in yellow.

Table S0: Tin-oxygen interatomic distances of **3** in the solid state. All bonds are in Å and the standard uncertainty on each is ±0.003 Å. Strong bonds (i.e., μ_3-O and covalent O_2CCF_3 bonds, ≤2.4 Å) are bolded and weak bonds (i.e., coordinative interactions, >2.4 Å) are normal weight. Intermolecular contacts are colored green.

	Sn1	Sn2	Sn3	Sn4	Sn5	Sn6
O1	**2.233**					
O2	2.755	2.636				
O3	**2.257**		2.685			
O4			2.880			
O5	**2.068**	**2.064**	**2.082**			
O6	2.973	2.276				
O7				2.570	2.635	
O8		**2.303**				
O9			**2.211**			
O10		2.739	**2.351**			
O11				**2.306**		2.859
O12				**2.075**	**2.078**	**2.099**
O13				**2.197**		
O14					**2.390**	
O15					2.457	
O16						**2.182**
O17				3.047		**2.325**
O18					**2.360**	2.805

Table S1. Selected crystallographic parameters for **3**.

Hexatin(II) di-μ_3-oxy-octakis-μ-trifluoroacetate (**3**)	
Identification code	CCDC 1885252
Empirical formula	$C_{16}F_{24}O_{18}Sn_6$
Formula weight	1648.3
Temperature	148(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 1 21/c 1
Unit cell dimensions	a = 13.2252(12) Å α = 90°
	b = 12.8538(11) Å β = 100.2660(10)°.
	c = 22.488(2) Å γ = 90°
Volume / Å^3	3761.6(6)
Z	4
ρ_{calc} / g cm^{-3}	2.911
μ / mm^{-1}	4.112
F(000)	3024
Crystal size / mm^3	0.115 × 0.14 × 0.07
θ range for data collection	1.565 to 27.995°
Index ranges	$-17 \le h \le 17$
	$-16 \le k \le 16$
	$-29 \le l \le 29$
Reflections collected	45 724
Independent reflections	9031 [R(int) = 0.0526]
Completeness to θ = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7458 and 0.6096
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9031 / 147 / 633
Goodness-of-fit on F^2	1.069
Final R indices [I > 2σ (I)]	R1 = 0.0310, ωR2 = 0.0575
R indices (all data)	R1 = 0.0444, ωR2 = 0.0622
Extinction coefficient	N/A
Largest diff. peak and hole / e Å^{-3}	0.966 and –1.166

Table S2. Bond lengths (in Å) for **3**.

Sn(1)-O(5)	2.068(3)	O(9)-C(7)	1.257(5)
Sn(1)-O(3)	2.257(3)	O(6)-C(5)	1.251(5)
Sn(1)-O(1)	2.232(3)	F(7)-C(6)	1.316(5)
/Sn(3)-O(5)	2.082(3)	F(17)-C(12)	1.325(5)
Sn(3)-O(10)	2.351(3)	O(4)-C(3)	1.209(5)
Sn(3)-O(9)	2.211(3)	O(1)-C(1)	1.255(5)
Sn(4)-O(12)	2.074(3)	F(16)-C(12)	1.315(5)
Sn(4)-O(13)	2.197(3)	F(13)-C(10)	1.317(5)
Sn(4)-O(11)	2.307(3)	O(2)-C(1)	1.236(5)
Sn(2)-O(5)	2.063(3)	O(14)-C(11)	1.237(5)
Sn(2)-O(8)	2.303(3)	F(18)-C(12)	1.327(5)
Sn(2)-O(6)	2.275(3)	O(17)-C(15)	1.244(5)
Sn(5)-O(12)	2.078(3)	F(15)-C(10)	1.298(5)
Sn(5)-O(18)#1	2.360(3)	F(9)-C(6)	1.308(5)
Sn(5)-O(14)	2.390(3)	F(8)-C(6)	1.342(6)
Sn(5)-O(15)	2.456(4)	O(16)-C(13)	1.230(6)
Sn(6)-O(12)	2.099(3)	C(1)-C(2)	1.538(6)
Sn(6)-O(17)	2.324(3)	C(3)-C(4)	1.538(6)
Sn(6)-O(16)	2.182(3)	C(9)-C(10)	1.543(6)
F(24)-C(16)	1.323(5)	C(5)-C(6)	1.528(6)
F(1)-C(2)	1.338(5)	O(15)-C(13)	1.233(6)
O(10)-C(9)	1.251(5)	C(15)-C(16)	1.548(6)
F(5)-C(4)	1.327(5)	C(12)-C(11)	1.539(6)
F(3)-C(2)	1.331(5)	C(7)-C(8)	1.511(6)
O(3)-C(3)	1.291(5)	C(13)-C(14)	1.499(7)
F(14)-C(10)	1.332(5)	F(12B)-C(8)	1.293(8)
F(22)-C(16)	1.326(5)	F(11B)-C(8)	1.265(7)
F(2)-C(2)	1.316(5)	F(10B)-C(8)	1.445(7)
O(13)-C(11)	1.255(5)	C(8)-F(12A)	1.269(10)
F(23)-C(16)	1.331(5)	C(8)-F(11A)	1.282(12)
F(6)-C(4)	1.337(5)	C(8)-F(10A)	1.535(10)
O(11)-C(9)	1.246(5)	F(21A)-C(14)	1.281(9)
O(18)-Sn(5)#2	2.360(3)	F(20A)-C(14)	1.294(8)
O(18)-C(15)	1.242(5)	F(19A)-C(14)	1.410(8)
F(4)-C(4)	1.326(5)	C(14)-F(20B)	1.347(14)
O(7)-C(5)	1.246(5)	C(14)-F(21B)	1.359(14)
O(8)-C(7)	1.242(5)	C(14)-F(19B)	1.572(12)

Symmetry transformations used to generate equivalent atoms: #1 ($-x + 2$, $-y - {}^{1}/_{2}$, $-z + {}^{3}/_{2}$); #2 ($-x + 2$, $-y + {}^{1}/_{2}$, $-z + {}^{3}/_{2}$).

Table S3. Bond angles (in °) for **3**.

O(5)-Sn(1)-O(3)	77.71(10)	F(2)-C(2)-C(1)	113.3(4)
O(5)-Sn(1)-O(1)	83.78(11)	F(14)-C(10)-C(9)	111.6(4)
O(1)-Sn(1)-O(3)	78.52(11)	F(13)-C(10)-F(14)	106.1(4)
O(5)-Sn(3)-O(10)	75.71(10)	F(13)-C(10)-C(9)	108.2(4)
O(5)-Sn(3)-O(9)	86.96(11)	F(15)-C(10)-F(14)	106.9(4)
O(9)-Sn(3)-O(10)	82.73(10)	F(15)-C(10)-F(13)	111.1(4)
O(12)-Sn(4)-O(13)	91.10(11)	F(15)-C(10)-C(9)	112.8(4)
O(12)-Sn(4)-O(11)	77.35(10)	C(13)-O(15)-Sn(5)	132.0(3)
O(13)-Sn(4)-O(11)	79.34(10)	O(18)-C(15)-O(17)	130.4(4)
O(5)-Sn(2)-O(8)	87.05(11)	O(18)-C(15)-C(16)	115.3(4)
O(5)-Sn(2)-O(6)	79.01(10)	O(17)-C(15)-C(16)	114.2(4)
O(6)-Sn(2)-O(8)	73.77(11)	F(17)-C(12)-F(18)	106.2(4)
O(12)-Sn(5)-O(18)#1	76.00(10)	F(17)-C(12)-C(11)	110.2(4)
O(12)-Sn(5)-O(14)	85.04(11)	F(16)-C(12)-F(17)	108.3(4)
O(12)-Sn(5)-O(15)	79.75(12)	F(16)-C(12)-F(18)	107.0(4)
O(18)#1-Sn(5)-O(14)	85.40(10)	F(16)-C(12)-C(11)	112.0(4)
O(18)#1-Sn(5)-O(15)	88.71(14)	F(18)-C(12)-C(11)	112.8(4)
O(14)-Sn(5)-O(15)	164.62(12)	F(7)-C(6)-F(8)	105.3(4)
O(12)-Sn(6)-O(17)	81.05(11)	F(7)-C(6)-C(5)	111.8(4)
O(12)-Sn(6)-O(16)	85.93(12)	F(9)-C(6)-F(7)	109.3(4)
O(16)-Sn(6)-O(17)	79.46(14)	F(9)-C(6)-F(8)	107.1(4)
Sn(1)-O(5)-Sn(3)	116.83(12)	F(9)-C(6)-C(5)	113.7(4)
Sn(2)-O(5)-Sn(1)	119.49(13)	F(8)-C(6)-C(5)	109.3(4)
Sn(2)-O(5)-Sn(3)	121.79(13)	F(24)-C(16)-F(22)	106.8(4)
Sn(4)-O(12)-Sn(5)	121.50(13)	F(24)-C(16)-F(23)	108.1(4)
Sn(4)-O(12)-Sn(6)	117.13(13)	F(24)-C(16)-C(15)	112.6(4)
Sn(5)-O(12)-Sn(6)	120.82(13)	F(22)-C(16)-F(23)	107.9(4)
C(9)-O(10)-Sn(3)	135.2(3)	F(22)-C(16)-C(15)	112.0(4)
C(3)-O(3)-Sn(1)	133.4(3)	F(23)-C(16)-C(15)	109.4(4)
C(11)-O(13)-Sn(4)	132.6(3)	O(13)-C(11)-C(12)	112.0(4)
C(9)-O(11)-Sn(4)	129.4(3)	O(14)-C(11)-O(13)	129.6(4)
C(15)-O(18)-Sn(5)#2	134.0(3)	O(14)-C(11)-C(12)	118.4(4)
C(7)-O(8)-Sn(2)	132.6(3)	O(8)-C(7)-O(9)	129.7(4)
C(7)-O(9)-Sn(3)	130.8(3)	O(8)-C(7)-C(8)	114.6(4)
C(5)-O(6)-Sn(2)	128.6(3)	O(9)-C(7)-C(8)	115.7(4)
C(1)-O(1)-Sn(1)	117.8(3)	O(16)-C(13)-O(15)	127.9(5)
C(11)-O(14)-Sn(5)	131.7(3)	O(16)-C(13)-C(14)	112.7(5)
C(15)-O(17)-Sn(6)	141.0(3)	O(15)-C(13)-C(14)	119.4(5)
C(13)-O(16)-Sn(6)	132.3(3)	C(7)-C(8)-F(10A)	100.9(5)

Table S3. Bond angles (in °) for **3**, *cont.*

O(1)-C(1)-C(2)	115.0(4)	F(12B)-C(8)-C(7)	114.1(7)
O(2)-C(1)-O(1)	126.8(4)	F(12B)-C(8)-F(10B)	101.3(6)
O(2)-C(1)-C(2)	118.2(4)	F(11B)-C(8)-C(7)	113.2(6)
O(3)-C(3)-C(4)	115.9(4)	F(11B)-C(8)-F(12B)	116.7(8)
O(4)-C(3)-O(3)	127.1(4)	F(11B)-C(8)-F(10B)	101.9(6)
O(4)-C(3)-C(4)	116.9(4)	F(10B)-C(8)-C(7)	107.7(4)
O(10)-C(9)-C(10)	116.2(4)	F(12A)-C(8)-C(7)	120.5(8)
O(11)-C(9)-O(10)	128.3(4)	F(12A)-C(8)-F(11A)	117.0(13)
O(11)-C(9)-C(10)	115.5(4)	F(12A)-C(8)-F(10A)	92.6(9)
O(7)-C(5)-O(6)	127.8(4)	F(11A)-C(8)-C(7)	120.0(13)
O(7)-C(5)-C(6)	118.3(4)	F(11A)-C(8)-F(10A)	92.2(11)
O(6)-C(5)-C(6)	113.8(4)	C(13)-C(14)-F(19B)	95.3(7)
F(5)-C(4)-F(6)	106.6(4)	F(21A)-C(14)-C(13)	112.5(8)
F(5)-C(4)-C(3)	111.9(4)	F(21A)-C(14)-F(20A)	115.9(9)
F(6)-C(4)-C(3)	113.2(4)	F(21A)-C(14)-F(19A)	100.1(8)
F(4)-C(4)-F(5)	107.4(4)	F(20A)-C(14)-C(13)	114.7(7)
F(4)-C(4)-F(6)	107.0(4)	F(20A)-C(14)-F(19A)	101.9(7)
F(4)-C(4)-C(3)	110.4(4)	F(19A)-C(14)-C(13)	110.0(5)
F(1)-C(2)-C(1)	110.8(4)	F(20B)-C(14)-C(13)	125.4(17)
F(3)-C(2)-F(1)	105.5(4)	F(20B)-C(14)-F(21B)	120(2)
F(3)-C(2)-C(1)	110.5(4)	F(20B)-C(14)-F(19B)	79.2(16)
F(2)-C(2)-F(1)	108.2(4)	F(21B)-C(14)-C(13)	112.0(18)
F(2)-C(2)-F(3)	108.2(4)	F(21B)-C(14)-F(19B)	79.9(13)

Symmetry transformations used to generate equivalent atoms: #1 ($-x + 2$, $-y - {}^{1}/_{2}$, $-z + {}^{3}/_{2}$); #2 ($-x + 2$, $-y + {}^{1}/_{2}$, $-z + {}^{3}/_{2}$).

Crystallography of tin(IV) tetrakis(trifluoroacetate) (5)

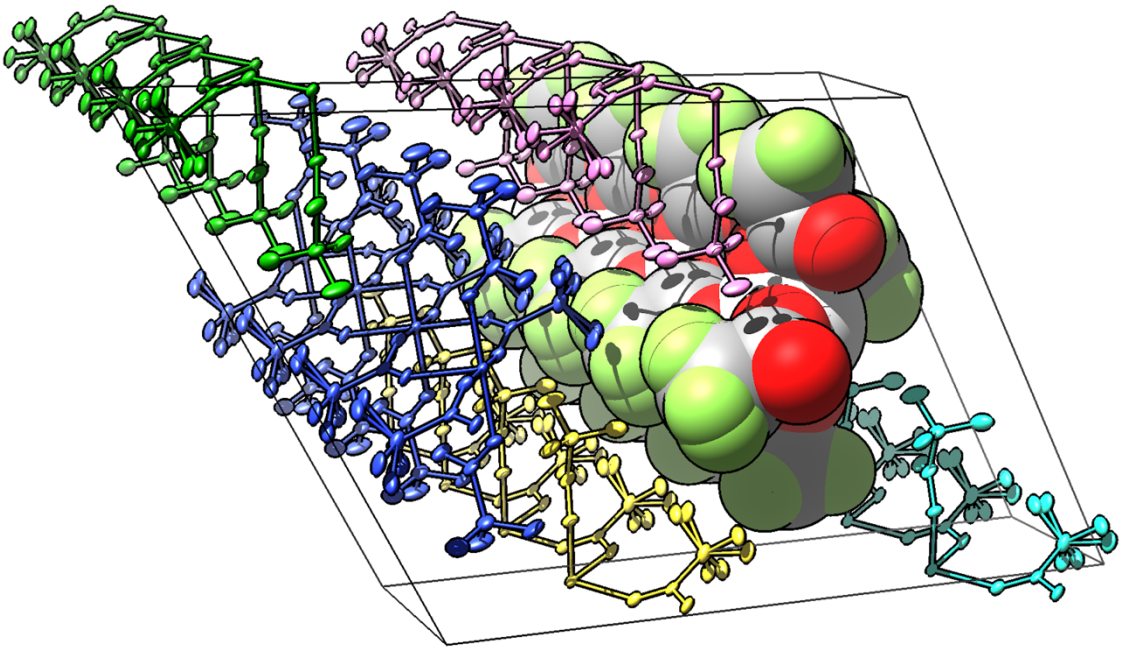

Figure S9. Crystal packing of a 1×4×1 supercell of **5**. Separate chains are depicted with thermal ellipsoids at 50% probability and single-coloured, except for one that is shown as a spacefilling diagram coloured by element (as in Figure S6).

Table S4. Selected crystallographic parameters for **5**.

Tin(IV) tetrakis(trifluoroacetate) (**5**)	
Identification code	CCDC 1885253
Empirical formula	$C_8F_{12}O_8Sn$
Formula weight / g mol^{-1}	570.77
Temperature / K	125.01
Wavelength / Å	0.71073
Crystal system	Monoclinic
Space group	C 1 2/c 1
Unit cell dimensions	a = 21.373(5) Å α = 90°
	b = 4.8415(11) Å β = 119.549(2)°
	c = 16.521(4) Å γ = 90°
Volume / Å^3	1487.1(6)
Z	4
ρ_{calc} / g cm^{-3}	2.549
μ / mm^{-1}	1.904
F(000)	1080
Crystal size / mm^3	0.25 × 0.11 × 0.09
θ range for data collection	2.191 to 29.027°
Index ranges	$-27 \le h \le 28$
	$-6 \le k \le 6$
	$-19 \le l \le 21$
Reflections collected	6260
Independent reflections	1875 [R(int) = 0.0425]
Completeness to θ = 25.242°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7458 and 0.6470
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1875 / 22 / 137
Goodness-of-fit on F^2	1.051
Final R indices [I > 2σ (I)]	R1 = 0.0328, ωR2 = 0.0648
R indices (all data)	R1 = 0.0564, ωR2 = 0.0707
Extinction coefficient	N/A
Largest diff. peak and hole / e Å^{-3}	0.829 and –0.748

Table S5 Bond lengths (in Å) for **5**.

C(1)-O(1)	1.314(4)
C(1)-C(2)	1.546(5)
C(1)-O(2)	1.200(4)
F(1)-C(2)	1.325(4)
O(1)-Sn(1)	1.991(2)
Sn(1)-O(1)#1	1.991(2)
Sn(1)-O(3)#1	2.074(2)
Sn(1)-O(3)	2.074(2)
Sn(1)-O(4)#2	2.079(2)
Sn(1)-O(4)#3	2.079(2)
C(2)-F(2)	1.320(4)
C(2)-F(3)	1.326(5)
C(3)-O(3)	1.242(4)
C(3)-C(4)	1.535(5)
C(3)-O(4)	1.258(4)
C(4)-F(4)	1.396(8)
C(4)-F(5)	1.362(7)
C(4)-F(6)	1.276(8)
C(4)-F(6A)	1.321(6)
C(4)-F(4A)	1.404(7)
C(4)-F(5A)	1.273(8)
O(4)-Sn(1)#4	2.079(2)

Table S6. Bond angles (in °) for **5**.

O(1)-C(1)-C(2)	110.9(3)	F(2)-C(2)-C(1)	109.5(3)
O(2)-C(1)-O(1)	128.5(4)	F(2)-C(2)-F(1)	108.4(3)
O(2)-C(1)-C(2)	120.6(4)	F(2)-C(2)-F(3)	108.1(4)
C(1)-O(1)-Sn(1)	123.6(2)	F(3)-C(2)-C(1)	112.6(3)
O(1)#1-Sn(1)-O(1)	180.00(6)	O(3)-C(3)-C(4)	118.0(3)
O(1)-Sn(1)-O(3)#1	90.11(9)	O(3)-C(3)-O(4)	125.7(3)
O(1)#1-Sn(1)-O(3)#1	89.89(9)	O(4)-C(3)-C(4)	116.3(3)
O(1)-Sn(1)-O(3)	89.90(9)	C(3)-O(3)-Sn(1)	150.6(2)
O(1)#1-Sn(1)-O(3)	90.10(9)	F(4)-C(4)-C(3)	104.4(4)
O(1)-Sn(1)-O(4)#3	92.12(10)	F(5)-C(4)-C(3)	110.3(4)
O(1)-Sn(1)-O(4)#2	87.88(10)	F(5)-C(4)-F(4)	102.9(5)
O(1)#1-Sn(1)-O(4)#3	87.88(10)	F(6)-C(4)-C(3)	114.7(4)
O(1)#1-Sn(1)-O(4)#2	92.12(10)	F(6)-C(4)-F(4)	111.7(6)
O(3)#1-Sn(1)-O(3)	180	F(6)-C(4)-F(5)	111.9(4)
O(3)-Sn(1)-O(4)#2	93.43(9)	F(6A)-C(4)-C(3)	112.6(3)
O(3)-Sn(1)-O(4)#3	86.57(9)	F(6A)-C(4)-F(4A)	105.5(4)
O(3)#1-Sn(1)-O(4)#2	86.58(9)	F(4A)-C(4)-C(3)	105.2(4)
O(3)#1-Sn(1)-O(4)#3	93.42(9)	F(5A)-C(4)-C(3)	115.0(4)
O(4)#2-Sn(1)-O(4)#3	180.00(14)	F(5A)-C(4)-F(6A)	113.2(4)
F(1)-C(2)-C(1)	110.4(3)	F(5A)-C(4)-F(4A)	104.0(5)
F(1)-C(2)-F(3)	107.7(3)	C(3)-O(4)-Sn(1)#4	127.7(2)

Symmetry transformations used to generate equivalent atoms:
#1 ($-x + {}^{3}/_{2}$, $-y + {}^{3}/_{2}$, $-z + 1$); #2 ($-x + {}^{3}/_{2}$, $-y + {}^{1}/_{2}$, $-z + 1$); #3 (x, $y + 1$, z); #4 (x, $y - 1$, z)

Crystallography of hexakis[tin(II) bis-μ-trifluoroacetate trimethylphosphine] (**1**←PMe_3)$_6$

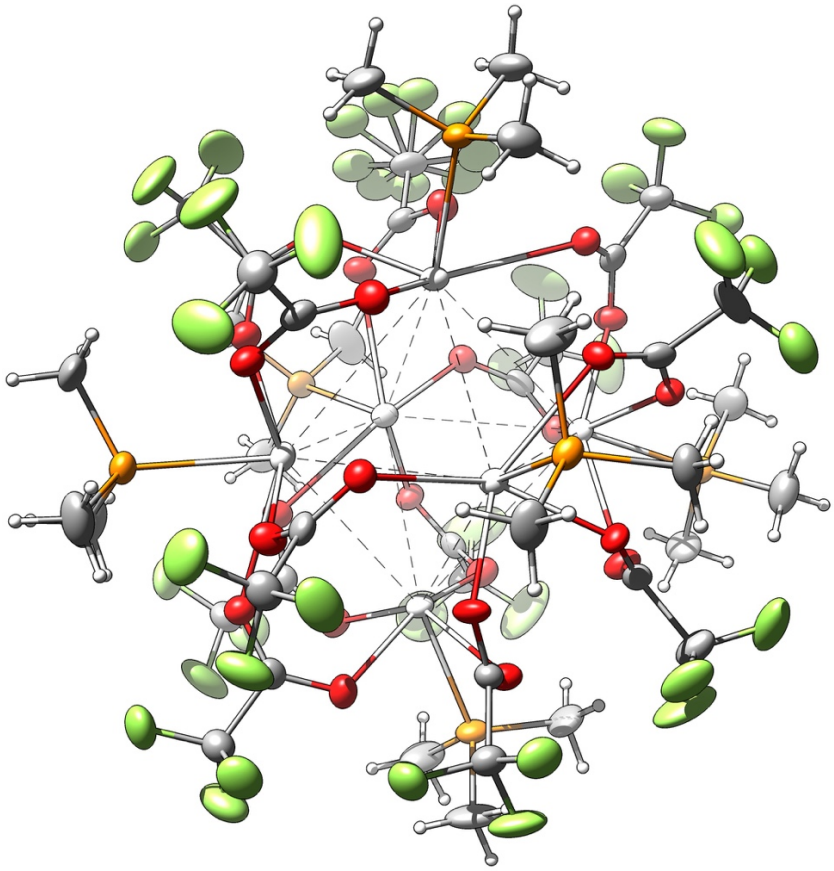

Figure S10. Molecular structure of (**1**←PMe_3)$_6$. Co-crystallized toluene has been omitted for clarity. Non-hydrogen atoms are depicted as ellipsoids at 50% probability, and hydrogens are depicted as spheres. Disordered CF_3 groups are shown. The closest Sn–Sn interatomic distances are shown as dashed lines to highlight geometry.

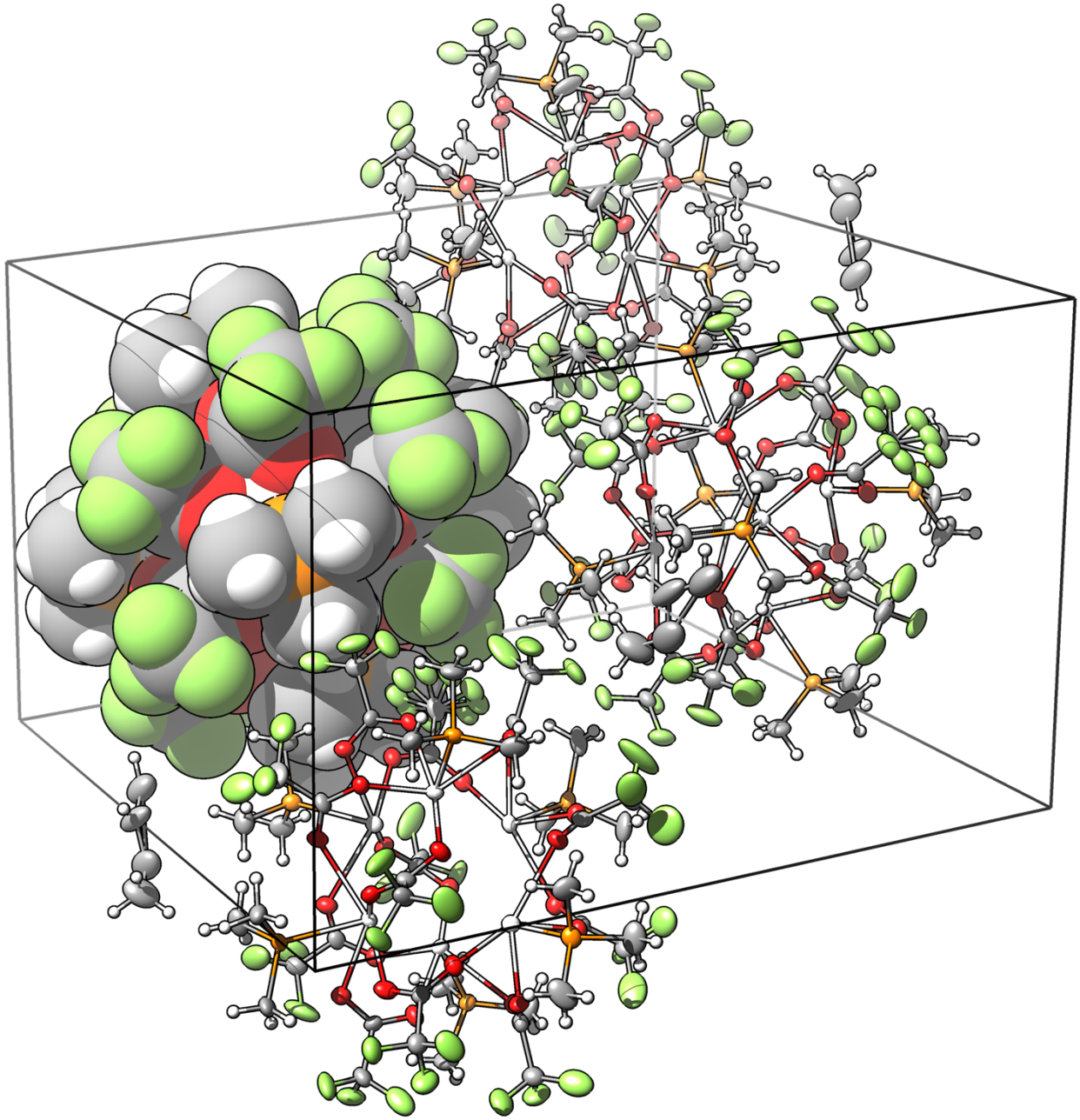

Figure S11. Crystal packing of (**1**←PMe_3)$_6$. Non-hydrogen atoms are depicted as ellipsoids at 50% probability, and hydrogens are depicted as spheres. Disordered CF_3 groups and co-crystallized toluene molecules are shown.

Table S7. Selected crystallographic parameters for (**1**←PMe_3)$_6$.

Hexakis(tin(II) bis-μ-trifluoroacetate trimethylphosphine) (**1**←PMe_3)$_6$	
Identification code	CCDC 1885254
Empirical formula	$C_{91}H_{115}F_{72}O_{48}P_{12}Sn_{12}$
Formula weight / g mol^{-1}	5140.74
Temperature / K	125(2)
Wavelength / Å	0.71073
Crystal system	Monoclinic
Space group	P 2_1/n
Unit cell dimensions	a = 15.150(3) Å α = 90°
	b = 24.993(5) Å β = 93.276(2)°
	c = 23.366(4) Å γ = 90°
Volume / Å^3	8833(3)
Z	2
ρ_{calc} / g cm^{-3}	1.933
μ / mm^{-1}	1.916
F(000)	4946
Crystal size / mm^3	0.220 × 0.210 × 0.130
range for data collection	1.194 to 27.000°.
Index ranges	$-19 \le h \le 19$
	$-31 \le k \le 31$
	$-29 \le l \le 29$
Reflections collected	101 717
Independent reflections	19 283 [R(int) = 0.0903]
Completeness to θ = 26.000°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7458 and 0.6194
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	19 283 / 19 / 1091
Goodness-of-fit on F^2	1.011
Final R indices [I > 2σ (I)]	R1 = 0.0382, ωR2 = 0.0780
R indices (all data)	R1 = 0.0644, ωR2 = 0.0897
Extinction coefficient	N/A
Largest diff. peak and hole / e Å^{-3}	1.087 and –1.140

Table S8. Bond lengths (in Å) for (**1**←PMe_3)$_6$.

Sn(1)-O(3)	2.216(3)	O(21)-C(36)	1.267(5)
Sn(1)-O(1)	2.221(3)	O(22)-C(36)	1.233(5)
Sn(1)-P(1)	2.6640(13)	O(23)-C(38)	1.261(5)
Sn(2)-O(5)	2.231(3)	O(24)-C(38)	1.233(5)
Sn(2)-O(7)	2.241(3)	C(1)-C(2)	1.529(6)
Sn(2)-P(2)	2.6699(13)	C(2)-F(1C)	1.22(3)
Sn(3)-O(9)	2.209(3)	C(2)-F(2C)	1.28(2)
Sn(3)-O(11)	2.235(3)	C(2)-F(3A)	1.318(9)
Sn(3)-P(3)	2.6473(13)	C(2)-F(3B)	1.332(13)
Sn(4)-O(15)	2.217(3)	C(2)-F(1A)	1.341(9)
Sn(4)-O(13)	2.223(3)	C(2)-F(2B)	1.343(13)
Sn(4)-P(4)	2.6583(13)	C(2)-F(1B)	1.354(14)
Sn(5)-O(19)	2.222(3)	C(2)-F(2A)	1.378(9)
Sn(5)-O(17)	2.250(3)	C(2)-F(3C)	1.41(3)
Sn(5)-P(5)	2.6590(13)	C(3)-C(4)	1.547(7)
Sn(6)-O(21)	2.222(3)	C(5)-H(5A)	0.98
Sn(6)-O(23)	2.259(3)	C(5)-H(5B)	0.98
Sn(6)-P(6)	2.6531(13)	C(5)-H(5C)	0.98
P(1)-C(5)	1.792(5)	C(6)-H(6A)	0.98
P(1)-C(6)	1.807(5)	C(6)-H(6B)	0.98
P(1)-C(7)	1.810(5)	C(6)-H(6C)	0.98
P(2)-C(13)	1.788(6)	C(7)-H(7A)	0.98
P(2)-C(14)	1.794(6)	C(7)-H(7B)	0.98
P(2)-C(12)	1.800(5)	C(7)-H(7C)	0.98
P(3)-C(21)	1.799(5)	C(8)-C(9)	1.548(7)
P(3)-C(19)	1.799(5)	C(10)-C(11)	1.531(6)
P(3)-C(20)	1.804(5)	C(12)-H(12A)	0.98
P(4)-C(27)	1.797(5)	C(12)-H(12B)	0.98
P(4)-C(28)	1.804(5)	C(12)-H(12C)	0.98
P(4)-C(26)	1.806(6)	C(13)-H(13A)	0.98
P(5)-C(34)	1.791(6)	C(13)-H(13B)	0.98
P(5)-C(35)	1.802(5)	C(13)-H(13C)	0.98
P(5)-C(33)	1.802(6)	C(14)-H(14A)	0.98
P(6)-C(42)	1.795(5)	C(14)-H(14B)	0.98
P(6)-C(41)	1.802(5)	C(14)-H(14C)	0.98
P(6)-C(40)	1.805(5)	C(15)-C(16)	1.535(6)
F(4)-C(4)	1.313(7)	C(17)-C(18)	1.529(6)

Table S8. Bond lengths (in Å) for (**1**←PMe_3)$_6$, *cont.*

F(5)-C(4)	1.329(7)	C(19)-H(19A)	0.98
F(6)-C(4)	1.330(6)	C(19)-H(19B)	0.98
F(7)-C(9)	1.315(6)	C(19)-H(19C)	0.98
F(8)-C(9)	1.313(6)	C(20)-H(20A)	0.98
F(9)-C(9)	1.324(6)	C(20)-H(20B)	0.98
F(10)-C(11)	1.329(6)	C(20)-H(20C)	0.98
F(11)-C(11)	1.333(6)	C(21)-H(21A)	0.98
F(12)-C(11)	1.324(5)	C(21)-H(21B)	0.98
F(13)-C(16)	1.312(6)	C(21)-H(21C)	0.98
F(14)-C(16)	1.322(5)	C(22)-C(23)	1.532(7)
F(15)-C(16)	1.313(6)	C(24)-C(25)	1.540(7)
F(16)-C(18)	1.337(5)	C(26)-H(26A)	0.98
F(17)-C(18)	1.332(6)	C(26)-H(26B)	0.98
F(18)-C(18)	1.322(5)	C(26)-H(26C)	0.98
F(19)-C(23)	1.332(6)	C(27)-H(27A)	0.98
F(20)-C(23)	1.322(6)	C(27)-H(27B)	0.98
F(21)-C(23)	1.328(6)	C(27)-H(27C)	0.98
F(22)-C(25)	1.321(6)	C(28)-H(28A)	0.98
F(23)-C(25)	1.323(6)	C(28)-H(28B)	0.98
F(24)-C(25)	1.331(6)	C(28)-H(28C)	0.98
F(25)-C(30)	1.321(7)	C(29)-C(30)	1.545(7)
F(26)-C(30)	1.326(7)	C(31)-C(32)	1.549(7)
F(27)-C(30)	1.333(6)	C(33)-H(33A)	0.98
F(28)-C(37)	1.313(7)	C(33)-H(33B)	0.98
F(29)-C(37)	1.324(6)	C(33)-H(33C)	0.98
F(30)-C(37)	1.331(6)	C(34)-H(34A)	0.98
F(31)-C(32)	1.309(7)	C(34)-H(34B)	0.98
F(32)-C(32)	1.293(7)	C(34)-H(34C)	0.98
F(33)-C(32)	1.309(6)	C(35)-H(35A)	0.98
F(34)-C(39)	1.328(5)	C(35)-H(35B)	0.98
F(35)-C(39)	1.345(6)	C(35)-H(35C)	0.98
F(36)-C(39)	1.326(6)	C(36)-C(37)	1.518(7)
O(1)-C(1)	1.261(5)	C(38)-C(39)	1.533(7)
O(2)-C(1)	1.226(5)	C(40)-H(40A)	0.98
O(3)-C(3)	1.253(6)	C(40)-H(40B)	0.98
O(4)-C(3)	1.237(6)	C(40)-H(40C)	0.98
O(5)-C(8)	1.260(6)	C(41)-H(41A)	0.98
O(6)-C(8)	1.228(6)	C(41)-H(41B)	0.98
O(7)-C(10)	1.261(5)	C(41)-H(41C)	0.98

Table S8. Bond lengths (in Å) for (**1**←PMe_3)$_6$, *cont.*

O(8)-C(10)	1.235(5)	C(42)-H(42A)	0.98
O(9)-C(15)	1.258(5)	C(42)-H(42B)	0.98
O(10)-C(15)	1.237(5)	C(42)-H(42C)	0.98
O(11)-C(17)	1.276(5)	C(50)-C(51)	1.298(12)
O(12)-C(17)	1.224(5)	C(50)-C(52)	1.408(13)
O(13)-C(22)	1.260(5)	C(50)-H(50)	0.95
O(14)-C(22)	1.226(5)	C(51)-C(52)#1	1.379(11)
O(15)-C(24)	1.273(5)	C(51)-H(51)	0.95
O(16)-C(24)	1.222(5)	C(52)-C(53)	1.193(15)
O(17)-C(29)	1.260(6)	C(52)-C(51)#1	1.379(11)
O(18)-C(29)	1.224(5)	C(53)-H(53A)	0.98
O(19)-C(31)	1.253(5)	C(53)-H(53B)	0.98
O(20)-C(31)	1.230(5)	C(53)-H(53C)	0.98

Symmetry transformations used to generate equivalent atoms: #1 (–*x* + 1, –y + 2, –*z* + 1)

Table S9. Bond angles (in °) for (**1**←PMe_3)$_6$.

O(3)-Sn(1)-O(1)	79.57(12)	P(1)-C(6)-H(6B)	109.5	H(26A)-C(26)-H(26B)	109.5
O(3)-Sn(1)-P(1)	80.80(9)	H(6A)-C(6)-H(6B)	109.5	P(4)-C(26)-H(26C)	109.5
O(1)-Sn(1)-P(1)	81.21(9)	P(1)-C(6)-H(6C)	109.5	H(26A)-C(26)-H(26C)	109.5
O(5)-Sn(2)-O(7)	79.88(11)	H(6A)-C(6)-H(6C)	109.5	H(26B)-C(26)-H(26C)	109.5
O(5)-Sn(2)-P(2)	78.52(9)	H(6B)-C(6)-H(6C)	109.5	P(4)-C(27)-H(27A)	109.5
O(7)-Sn(2)-P(2)	82.12(9)	P(1)-C(7)-H(7A)	109.5	P(4)-C(27)-H(27B)	109.5
O(9)-Sn(3)-O(11)	79.76(11)	P(1)-C(7)-H(7B)	109.5	H(27A)-C(27)-H(27B)	109.5
O(9)-Sn(3)-P(3)	80.83(8)	H(7A)-C(7)-H(7B)	109.5	P(4)-C(27)-H(27C)	109.5
O(11)-Sn(3)-P(3)	82.54(9)	P(1)-C(7)-H(7C)	109.5	H(27A)-C(27)-H(27C)	109.5
O(15)-Sn(4)-O(13)	80.12(12)	H(7A)-C(7)-H(7C)	109.5	H(27B)-C(27)-H(27C)	109.5
O(15)-Sn(4)-P(4)	80.57(9)	H(7B)-C(7)-H(7C)	109.5	P(4)-C(28)-H(28A)	109.5
O(13)-Sn(4)-P(4)	82.28(8)	O(6)-C(8)-O(5)	130.4(4)	P(4)-C(28)-H(28B)	109.5
O(19)-Sn(5)-O(17)	79.30(12)	O(6)-C(8)-C(9)	117.4(4)	H(28A)-C(28)-H(28B)	109.5
O(19)-Sn(5)-P(5)	77.88(9)	O(5)-C(8)-C(9)	112.2(4)	P(4)-C(28)-H(28C)	109.5
O(17)-Sn(5)-P(5)	82.53(9)	F(8)-C(9)-F(7)	107.5(5)	H(28A)-C(28)-H(28C)	109.5
O(21)-Sn(6)-O(23)	78.53(11)	F(8)-C(9)-F(9)	107.0(5)	H(28B)-C(28)-H(28C)	109.5
O(21)-Sn(6)-P(6)	79.89(8)	F(7)-C(9)-F(9)	106.7(5)	O(18)-C(29)-O(17)	129.4(4)
O(23)-Sn(6)-P(6)	82.98(9)	F(8)-C(9)-C(8)	112.5(4)	O(18)-C(29)-C(30)	118.0(5)
C(5)-P(1)-C(6)	105.3(3)	F(7)-C(9)-C(8)	112.9(4)	O(17)-C(29)-C(30)	112.5(4)
C(5)-P(1)-C(7)	105.6(3)	F(9)-C(9)-C(8)	110.0(4)	F(25)-C(30)-F(26)	107.1(5)
C(6)-P(1)-C(7)	104.7(3)	O(8)-C(10)-O(7)	129.5(4)	F(25)-C(30)-F(27)	107.6(5)
C(5)-P(1)-Sn(1)	112.66(18)	O(8)-C(10)-C(11)	117.2(4)	F(26)-C(30)-F(27)	107.0(5)
C(6)-P(1)-Sn(1)	113.95(18)	O(7)-C(10)-C(11)	113.3(4)	F(25)-C(30)-C(29)	112.3(5)
C(7)-P(1)-Sn(1)	113.82(18)	F(12)-C(11)-F(10)	106.7(4)	F(26)-C(30)-C(29)	112.9(5)
C(13)-P(2)-C(14)	105.0(3)	F(12)-C(11)-F(11)	106.6(4)	F(27)-C(30)-C(29)	109.8(4)
C(13)-P(2)-C(12)	104.6(3)	F(10)-C(11)-F(11)	106.9(4)	O(20)-C(31)-O(19)	130.4(4)
C(14)-P(2)-C(12)	105.4(3)	F(12)-C(11)-C(10)	113.6(4)	O(20)-C(31)-C(32)	116.8(4)
C(13)-P(2)-Sn(2)	111.2(2)	F(10)-C(11)-C(10)	110.5(4)	O(19)-C(31)-C(32)	112.7(4)
C(14)-P(2)-Sn(2)	115.8(2)	F(11)-C(11)-C(10)	112.2(4)	F(32)-C(32)-F(33)	109.3(6)
C(12)-P(2)-Sn(2)	113.9(2)	P(2)-C(12)-H(12A)	109.5	F(32)-C(32)-F(31)	107.4(5)
C(21)-P(3)-C(19)	104.8(2)	P(2)-C(12)-H(12B)	109.5	F(33)-C(32)-F(31)	105.5(6)
C(21)-P(3)-C(20)	106.2(3)	H(12A)-C(12)-H(12B)	109.5	F(32)-C(32)-C(31)	113.1(5)
C(19)-P(3)-C(20)	104.8(3)	P(2)-C(12)-H(12C)	109.5	F(33)-C(32)-C(31)	111.2(5)
C(21)-P(3)-Sn(3)	115.51(18)	H(12A)-C(12)-H(12C)	109.5	F(31)-C(32)-C(31)	109.9(5)
C(19)-P(3)-Sn(3)	113.91(17)	H(12B)-C(12)-H(12C)	109.5	P(5)-C(33)-H(33A)	109.5
C(20)-P(3)-Sn(3)	110.75(17)	P(2)-C(13)-H(13A)	109.5	P(5)-C(33)-H(33B)	109.5
C(27)-P(4)-C(28)	104.9(3)	P(2)-C(13)-H(13B)	109.5	H(33A)-C(33)-H(33B)	109.5
C(27)-P(4)-C(26)	105.4(3)	H(13A)-C(13)-H(13B)	109.5	P(5)-C(33)-H(33C)	109.5
C(28)-P(4)-C(26)	105.9(3)	P(2)-C(13)-H(13C)	109.5	H(33A)-C(33)-H(33C)	109.5

Table S9. Bond angles (in °) for (**1**←PMe_3)$_6$, *cont.*

C(27)-P(4)-Sn(4)	114.43(18)	H(13A)-C(13)-H(13C)	109.5	H(33B)-C(33)-H(33C)	109.5
C(28)-P(4)-Sn(4)	113.43(19)	H(13B)-C(13)-H(13C)	109.5	P(5)-C(34)-H(34A)	109.5
C(26)-P(4)-Sn(4)	112.01(18)	P(2)-C(14)-H(14A)	109.5	P(5)-C(34)-H(34B)	109.5
C(34)-P(5)-C(35)	105.1(3)	P(2)-C(14)-H(14B)	109.5	H(34A)-C(34)-H(34B)	109.5
C(34)-P(5)-C(33)	106.3(3)	H(14A)-C(14)-H(14B)	109.5	P(5)-C(34)-H(34C)	109.5
C(35)-P(5)-C(33)	104.3(3)	P(2)-C(14)-H(14C)	109.5	H(34A)-C(34)-H(34C)	109.5
C(34)-P(5)-Sn(5)	113.4(2)	H(14A)-C(14)-H(14C)	109.5	H(34B)-C(34)-H(34C)	109.5
C(35)-P(5)-Sn(5)	115.15(18)	H(14B)-C(14)-H(14C)	109.5	P(5)-C(35)-H(35A)	109.5
C(33)-P(5)-Sn(5)	111.75(19)	O(10)-C(15)-O(9)	129.8(4)	P(5)-C(35)-H(35B)	109.5
C(42)-P(6)-C(41)	105.8(3)	O(10)-C(15)-C(16)	116.6(4)	H(35A)-C(35)-H(35B)	109.5
C(42)-P(6)-C(40)	105.2(3)	O(9)-C(15)-C(16)	113.5(4)	P(5)-C(35)-H(35C)	109.5
C(41)-P(6)-C(40)	104.3(3)	F(13)-C(16)-F(15)	107.5(4)	H(35A)-C(35)-H(35C)	109.5
C(42)-P(6)-Sn(6)	111.37(18)	F(13)-C(16)-F(14)	107.2(4)	H(35B)-C(35)-H(35C)	109.5
C(41)-P(6)-Sn(6)	115.39(18)	F(15)-C(16)-F(14)	105.8(4)	O(22)-C(36)-O(21)	130.1(4)
C(40)-P(6)-Sn(6)	113.94(18)	F(13)-C(16)-C(15)	110.4(4)	O(22)-C(36)-C(37)	118.0(4)
C(1)-O(1)-Sn(1)	119.7(3)	F(15)-C(16)-C(15)	113.4(4)	O(21)-C(36)-C(37)	111.8(4)
C(3)-O(3)-Sn(1)	127.3(3)	F(14)-C(16)-C(15)	112.2(4)	F(28)-C(37)-F(29)	107.0(5)
C(8)-O(5)-Sn(2)	125.0(3)	O(12)-C(17)-O(11)	128.3(4)	F(28)-C(37)-F(30)	105.4(5)
C(10)-O(7)-Sn(2)	125.7(3)	O(12)-C(17)-C(18)	119.5(4)	F(29)-C(37)-F(30)	105.9(5)
C(15)-O(9)-Sn(3)	130.8(3)	O(11)-C(17)-C(18)	112.2(4)	F(28)-C(37)-C(36)	113.3(5)
C(17)-O(11)-Sn(3)	122.7(3)	F(18)-C(18)-F(17)	108.4(4)	F(29)-C(37)-C(36)	113.1(4)
C(22)-O(13)-Sn(4)	125.5(3)	F(18)-C(18)-F(16)	106.7(4)	F(30)-C(37)-C(36)	111.6(4)
C(24)-O(15)-Sn(4)	118.6(3)	F(17)-C(18)-F(16)	107.1(4)	O(24)-C(38)-O(23)	129.6(4)
C(29)-O(17)-Sn(5)	125.2(3)	F(18)-C(18)-C(17)	112.6(4)	O(24)-C(38)-C(39)	117.4(4)
C(31)-O(19)-Sn(5)	125.7(3)	F(17)-C(18)-C(17)	110.8(4)	O(23)-C(38)-C(39)	113.0(4)
C(36)-O(21)-Sn(6)	125.8(3)	F(16)-C(18)-C(17)	111.1(4)	F(36)-C(39)-F(34)	107.4(4)
C(38)-O(23)-Sn(6)	123.4(3)	P(3)-C(19)-H(19A)	109.5	F(36)-C(39)-F(35)	106.7(4)
O(2)-C(1)-O(1)	129.2(4)	P(3)-C(19)-H(19B)	109.5	F(34)-C(39)-F(35)	105.9(4)
O(2)-C(1)-C(2)	117.7(4)	H(19A)-C(19)-H(19B)	109.5	F(36)-C(39)-C(38)	111.9(4)
O(1)-C(1)-C(2)	113.0(4)	P(3)-C(19)-H(19C)	109.5	F(34)-C(39)-C(38)	113.3(4)
F(1C)-C(2)-F(2C)	109.3(18)	H(19A)-C(19)-H(19C)	109.5	F(35)-C(39)-C(38)	111.2(4)
F(3A)-C(2)-F(1A)	108.9(6)	H(19B)-C(19)-H(19C)	109.5	P(6)-C(40)-H(40A)	109.5
F(3B)-C(2)-F(2B)	104.9(7)	P(3)-C(20)-H(20A)	109.5	P(6)-C(40)-H(40B)	109.5
F(3B)-C(2)-F(1B)	106.7(8)	P(3)-C(20)-H(20B)	109.5	H(40A)-C(40)-H(40B)	109.5
F(2B)-C(2)-F(1B)	107.0(8)	H(20A)-C(20)-H(20B)	109.5	P(6)-C(40)-H(40C)	109.5
F(3A)-C(2)-F(2A)	106.9(6)	P(3)-C(20)-H(20C)	109.5	H(40A)-C(40)-H(40C)	109.5
F(1A)-C(2)-F(2A)	106.3(6)	H(20A)-C(20)-H(20C)	109.5	H(40B)-C(40)-H(40C)	109.5
F(1C)-C(2)-F(3C)	104.0(16)	H(20B)-C(20)-H(20C)	109.5	P(6)-C(41)-H(41A)	109.5
F(2C)-C(2)-F(3C)	102.8(16)	P(3)-C(21)-H(21A)	109.5	P(6)-C(41)-H(41B)	109.5

Table S9. Bond angles (in °) for (**1**←PMe_3)$_6$, *cont.*

F(1C)-C(2)-C(1)	117.8(13)	P(3)-C(21)-H(21B)	109.5	H(41A)-C(41)-H(41B)	109.5
F(2C)-C(2)-C(1)	115.1(10)	H(21A)-C(21)-H(21B)	109.5	P(6)-C(41)-H(41C)	109.5
F(3A)-C(2)-C(1)	111.7(5)	P(3)-C(21)-H(21C)	109.5	H(41A)-C(41)-H(41C)	109.5
F(3B)-C(2)-C(1)	112.5(6)	H(21A)-C(21)-H(21C)	109.5	H(41B)-C(41)-H(41C)	109.5
F(1A)-C(2)-C(1)	113.3(5)	H(21B)-C(21)-H(21C)	109.5	P(6)-C(42)-H(42A)	109.5
F(2B)-C(2)-C(1)	111.7(6)	O(14)-C(22)-O(13)	130.4(4)	P(6)-C(42)-H(42B)	109.5
F(1B)-C(2)-C(1)	113.5(6)	O(14)-C(22)-C(23)	117.5(4)	H(42A)-C(42)-H(42B)	109.5
F(2A)-C(2)-C(1)	109.6(5)	O(13)-C(22)-C(23)	112.0(4)	P(6)-C(42)-H(42C)	109.5
F(3C)-C(2)-C(1)	106.2(10)	F(20)-C(23)-F(21)	107.4(4)	H(42A)-C(42)-H(42C)	109.5
O(4)-C(3)-O(3)	130.2(4)	F(20)-C(23)-F(19)	106.5(5)	H(42B)-C(42)-H(42C)	109.5
O(4)-C(3)-C(4)	118.2(5)	F(21)-C(23)-F(19)	105.9(4)	C(51)-C(50)-C(52)	121.1(9)
O(3)-C(3)-C(4)	111.5(4)	F(20)-C(23)-C(22)	112.0(4)	C(51)-C(50)-H(50)	119.4
F(4)-C(4)-F(5)	109.1(5)	F(21)-C(23)-C(22)	111.3(4)	C(52)-C(50)-H(50)	119.4
F(4)-C(4)-F(6)	107.4(5)	F(19)-C(23)-C(22)	113.3(4)	C(50)-C(51)-C(52)#1	120.4(11)
F(5)-C(4)-F(6)	107.5(5)	O(16)-C(24)-O(15)	128.5(4)	C(50)-C(51)-H(51)	119.8
F(4)-C(4)-C(3)	111.3(5)	O(16)-C(24)-C(25)	118.9(4)	C(52)#1-C(51)-H(51)	119.8
F(5)-C(4)-C(3)	109.0(4)	O(15)-C(24)-C(25)	112.6(4)	C(53)-C(52)-C(51)#1	120.9(15)
F(6)-C(4)-C(3)	112.4(5)	F(22)-C(25)-F(23)	107.7(4)	C(53)-C(52)-C(50)	120.6(13)
P(1)-C(5)-H(5A)	109.5	F(22)-C(25)-F(24)	107.8(4)	C(51)#1-C(52)-C(50)	118.5(10)
P(1)-C(5)-H(5B)	109.5	F(23)-C(25)-F(24)	106.4(4)	C(52)-C(53)-H(53A)	109.5
H(5A)-C(5)-H(5B)	109.5	F(22)-C(25)-C(24)	111.8(4)	C(52)-C(53)-H(53B)	109.5
P(1)-C(5)-H(5C)	109.5	F(23)-C(25)-C(24)	112.4(4)	H(53A)-C(53)-H(53B)	109.5
H(5A)-C(5)-H(5C)	109.5	F(24)-C(25)-C(24)	110.5(4)	C(52)-C(53)-H(53C)	109.5
H(5B)-C(5)-H(5C)	109.5	P(4)-C(26)-H(26A)	109.5	H(53A)-C(53)-H(53C)	109.5
P(1)-C(6)-H(6A)	109.5	P(4)-C(26)-H(26B)	109.5	H(53B)-C(53)-H(53C)	109.5

Crystallography of tin(IV) tetrakis(trifluoroacetate)-bis-*trans*-diethyl ether [**6**←$(OEt_2)_2$]

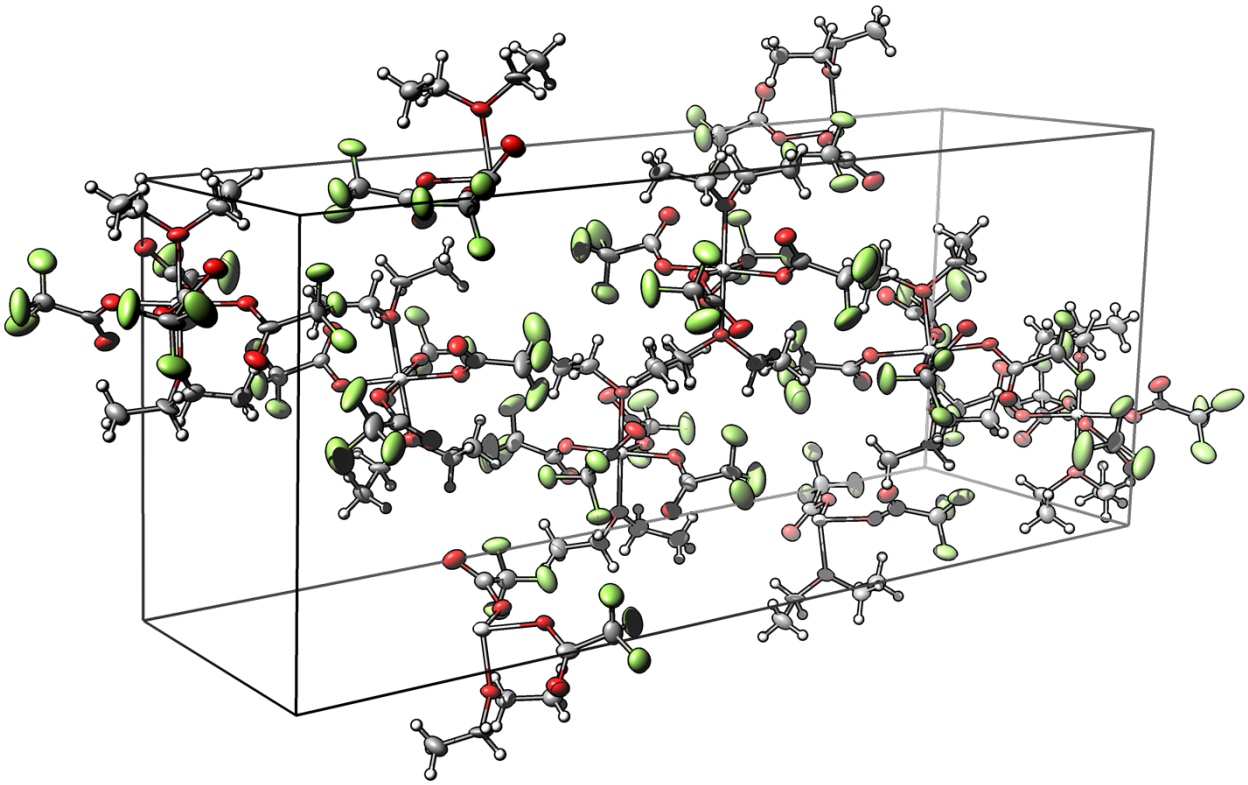

Figure S12. Unit cell of **6**←$(OEt_2)_2$. Non-hydrogen atoms are depicted as ellipsoids at 50% probability and hydrogens are depicted as spheres.

Table S10. Selected crystallographic parameters for **6**←$(OEt_2)_2$.

Tin(IV) tetrakis(trifluoroacetate)-bis-*trans*-diethyl ether [**6**←$(OEt_2)_2$]	
Identification code	CCDC 1885255
Empirical formula	$C_{16}H_{20}F_{12}O_{10}Sn$
Formula weight / g mol^{-1}	719.01
Temperature / K	125(2)
Wavelength / Å	0.71073
Crystal system	Monoclinic
Space group	P 1 2/c 1
Unit cell dimensions	a = 14.152(2) Å α = 90° b = 11.0124(18) Å β = 93.2° c = 32.890(6) Å γ = 90°
Volume / Å^3	5117.5(15)
Z	8
ρ_{calc} / g cm^{-3}	1.866
μ / mm^{-1}	1.133
F(000)	2832
Crystal size / mm^3	0.12 × 0.11 × 0.08
θ range for data collection	1.240 to 25.374°
Index ranges	$-16 \le h \le 17$ $-13 \le k \le 13$ $-39 \le l \le 39$
Reflections collected	50 039
Independent reflections	9380 [R(int) = 0.1181]
Completeness to θ = 26.000°	99.9%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7452 and 0.6372
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9380 / 60 / 712
Goodness-of-fit on F^2	1.026
Final R indices [I > 2σ (I)]	R1 = 0.0587, ωR2 = 0.1304
R indices (all data)	R1 = 0.1281, ωR2 = 0.1605
Extinction coefficient	N/A
Largest diff. peak and hole / e Å^{-3}	0.827 and –1.047

Table S11. Bond lengths (in Å) for compound **6**←$(OEt_2)_2$.

C(1)-O(1)	1.313(8)	C(11)-H(11B)	0.97	C(22)-H(22B)	0.96
C(1)-C(2)	1.506(11)	C(11)-C(12)	1.509(10)	C(22)-H(22C)	0.96
C(1)-O(2)	1.212(9)	C(12)-H(12A)	0.96	C(23)-H(23A)	0.97
F(1)-C(2)	1.320(9)	C(12)-H(12B)	0.96	C(23)-H(23B)	0.97
O(1)-Sn(1)	2.024(5)	C(12)-H(12C)	0.96	C(23)-C(24)	1.486(11)
Sn(1)-O(3)	2.030(5)	C(13)-H(13A)	0.96	C(24)-H(24A)	0.96
Sn(1)-O(5)	2.039(5)	C(13)-H(13B)	0.96	C(24)-H(24B)	0.96
Sn(1)-O(7)	2.016(5)	C(13)-H(13C)	0.96	C(24)-H(24C)	0.96
Sn(1)-O(9)	2.121(5)	C(13)-C(14)	1.490(10)	Sn(3)-O(16)	2.014(5)
Sn(1)-O(10)	2.126(5)	C(14)-H(14A)	0.97	Sn(3)-O(16)#2	2.014(5)
C(2)-F(2)	1.311(9)	C(14)-H(14B)	0.97	Sn(3)-O(18)#2	2.022(5)
C(2)-F(3)	1.304(9)	C(15)-H(15A)	0.97	Sn(3)-O(18)	2.022(5)
C(3)-O(3)	1.306(9)	C(15)-H(15B)	0.97	Sn(3)-O(20)#2	2.117(5)
C(3)-C(4)	1.542(11)	C(15)-C(16)	1.504(11)	Sn(3)-O(20)	2.117(5)
C(3)-O(4)	1.195(9)	C(16)-H(16A)	0.96	O(16)-C(25)	1.316(9)
C(4)-F(4)	1.295(9)	C(16)-H(16B)	0.96	O(17)-C(25)	1.201(9)
C(4)-F(5)	1.309(9)	C(16)-H(16C)	0.96	O(18)-C(27)	1.317(8)
C(4)-F(6)	1.298(10)	Sn(2)-O(11)#1	2.018(5)	F(19)-C(26)	1.414(13)
C(5)-O(5)	1.310(8)	Sn(2)-O(11)	2.018(5)	O(19)-C(27)	1.197(9)
C(5)-C(6)	1.520(11)	Sn(2)-O(13)#1	2.014(5)	F(20)-C(26)	1.238(11)
C(5)-O(6)	1.209(9)	Sn(2)-O(13)	2.014(5)	O(20)-C(29)	1.478(8)
C(6)-F(7)	1.324(8)	Sn(2)-O(15)#1	2.127(5)	O(20)-C(31)	1.479(8)
C(6)-F(8)	1.328(8)	Sn(2)-O(15)	2.127(5)	F(21)-C(26)	1.283(10)
C(6)-F(9)	1.347(9)	O(11)-C(17)	1.301(9)	F(22)-C(28)	1.330(9)
C(7)-O(7)	1.311(9)	O(12)-C(17)	1.204(9)	F(23)-C(28)	1.309(10)
C(7)-C(8)	1.504(11)	F(13)-C(18)	1.322(9)	F(24)-C(28)	1.332(10)
C(7)-O(8)	1.211(9)	O(13)-C(19)	1.310(8)	C(25)-C(26)	1.505(12)
C(8)-F(10)	1.282(10)	F(14)-C(18)	1.347(9)	C(27)-C(28)	1.517(11)
C(8)-F(11)	1.292(10)	O(14)-C(19)	1.203(9)	C(29)-H(29A)	0.97
C(8)-F(12)	1.306(11)	F(15)-C(18)	1.315(9)	C(29)-H(29B)	0.97
C(9)-H(9A)	0.97	O(15)-C(21)	1.476(8)	C(29)-C(30)	1.501(10)
C(9)-H(9B)	0.97	O(15)-C(23)	1.468(8)	C(30)-H(30A)	0.96
C(9)-O(9)	1.468(8)	F(16)-C(20)	1.318(9)	C(30)-H(30B)	0.96
C(9)-C(10)	1.490(10)	C(17)-C(18)	1.535(11)	C(30)-H(30C)	0.96
O(9)-C(11)	1.481(8)	F(17)-C(20)	1.325(9)	C(31)-H(31A)	0.97
C(10)-H(10A)	0.96	F(18)-C(20)	1.327(10)	C(31)-H(31B)	0.97
C(10)-H(10B)	0.96	C(19)-C(20)	1.517(11)	C(31)-C(32)	1.487(10)
C(10)-H(10C)	0.96	C(21)-H(21A)	0.97	C(32)-H(32A)	0.96
O(10)-C(14)	1.495(8)	C(21)-H(21B)	0.97	C(32)-H(32B)	0.96
O(10)-C(15)	1.476(8)	C(21)-C(22)	1.500(10)	C(32)-H(32C)	0.96
C(11)-H(11A)	0.97	C(22)-H(22A)	0.96		

Symmetry transformations used to generate equivalent atoms: #1 ($-x$, y, $-z + 3/2$); #2 ($-x + 1$, y, $-z + 3/2$).

Table S12. Bond angles (in °) for compound **6**←$(OEt_2)_2$.

O(1)-C(1)-C(2)	111.4(7)	F(7)-C(6)-C(5)	113.8(7)	C(12)-C(11)-H(11B)	109.6
O(2)-C(1)-O(1)	127.0(8)	F(7)-C(6)-F(8)	107.7(7)	C(11)-C(12)-H(12A)	109.5
O(2)-C(1)-C(2)	121.6(7)	F(7)-C(6)-F(9)	106.3(6)	C(11)-C(12)-H(12B)	109.5
C(1)-O(1)-Sn(1)	125.8(5)	F(8)-C(6)-C(5)	111.6(6)	C(11)-C(12)-H(12C)	109.5
O(1)-Sn(1)-O(3)	84.9(2)	F(8)-C(6)-F(9)	106.7(7)	H(12A)-C(12)-H(12B)	109.5
O(1)-Sn(1)-O(5)	177.7(2)	F(9)-C(6)-C(5)	110.4(6)	H(12A)-C(12)-H(12C)	109.5
O(1)-Sn(1)-O(9)	88.32(19)	O(7)-C(7)-C(8)	112.3(7)	H(12B)-C(12)-H(12C)	109.5
O(1)-Sn(1)-O(10)	91.06(19)	O(8)-C(7)-O(7)	128.1(7)	H(13A)-C(13)-H(13B)	109.5
O(3)-Sn(1)-O(5)	95.19(19)	O(8)-C(7)-C(8)	119.6(8)	H(13A)-C(13)-H(13C)	109.5
O(3)-Sn(1)-O(9)	91.35(19)	C(7)-O(7)-Sn(1)	124.8(5)	H(13B)-C(13)-H(13C)	109.5
O(3)-Sn(1)-O(10)	88.57(19)	F(10)-C(8)-C(7)	114.3(8)	C(14)-C(13)-H(13A)	109.5
O(5)-Sn(1)-O(9)	89.38(19)	F(10)-C(8)-F(11)	106.7(9)	C(14)-C(13)-H(13B)	109.5
O(5)-Sn(1)-O(10)	91.24(19)	F(10)-C(8)-F(12)	106.9(9)	C(14)-C(13)-H(13C)	109.5
O(7)-Sn(1)-O(1)	96.2(2)	F(11)-C(8)-C(7)	113.2(8)	O(10)-C(14)-H(14A)	109.5
O(7)-Sn(1)-O(3)	177.2(2)	F(11)-C(8)-F(12)	102.5(8)	O(10)-C(14)-H(14B)	109.5
O(7)-Sn(1)-O(5)	83.78(19)	F(12)-C(8)-C(7)	112.5(8)	C(13)-C(14)-O(10)	110.6(6)
O(7)-Sn(1)-O(9)	91.20(19)	H(9A)-C(9)-H(9B)	108	C(13)-C(14)-H(14A)	109.5
O(7)-Sn(1)-O(10)	88.89(19)	O(9)-C(9)-H(9A)	109.3	C(13)-C(14)-H(14B)	109.5
O(9)-Sn(1)-O(10)	179.4(2)	O(9)-C(9)-H(9B)	109.3	H(14A)-C(14)-H(14B)	108.1
F(1)-C(2)-C(1)	111.4(7)	O(9)-C(9)-C(10)	111.6(6)	O(10)-C(15)-H(15A)	109.6
F(2)-C(2)-C(1)	110.6(7)	C(10)-C(9)-H(9A)	109.3	O(10)-C(15)-H(15B)	109.6
F(2)-C(2)-F(1)	105.5(7)	C(10)-C(9)-H(9B)	109.3	O(10)-C(15)-C(16)	110.1(6)
F(3)-C(2)-C(1)	114.4(7)	C(9)-O(9)-Sn(1)	123.8(5)	H(15A)-C(15)-H(15B)	108.2
F(3)-C(2)-F(1)	106.9(7)	C(9)-O(9)-C(11)	112.4(6)	C(16)-C(15)-H(15A)	109.6
F(3)-C(2)-F(2)	107.5(7)	C(11)-O(9)-Sn(1)	123.8(4)	C(16)-C(15)-H(15B)	109.6
O(3)-C(3)-C(4)	110.2(7)	C(9)-C(10)-H(10A)	109.5	C(15)-C(16)-H(16A)	109.5
O(4)-C(3)-O(3)	128.2(8)	C(9)-C(10)-H(10B)	109.5	C(15)-C(16)-H(16B)	109.5
O(4)-C(3)-C(4)	121.6(8)	C(9)-C(10)-H(10C)	109.5	C(15)-C(16)-H(16C)	109.5
C(3)-O(3)-Sn(1)	124.2(5)	H(10A)-C(10)-H(10B)	109.5	H(16A)-C(16)-H(16B)	109.5
F(4)-C(4)-C(3)	112.0(7)	H(10A)-C(10)-H(10C)	109.5	H(16A)-C(16)-H(16C)	109.5
F(4)-C(4)-F(5)	106.6(8)	H(10B)-C(10)-H(10C)	109.5	H(16B)-C(16)-H(16C)	109.5
F(4)-C(4)-F(6)	109.4(8)	C(14)-O(10)-Sn(1)	123.4(4)	O(11)-Sn(2)-O(11)#1	97.6(3)
F(5)-C(4)-C(3)	110.0(7)	C(15)-O(10)-Sn(1)	124.0(4)	O(11)#1-Sn(2)-O(15)	92.25(19)
F(6)-C(4)-C(3)	112.1(7)	C(15)-O(10)-C(14)	112.7(6)	O(11)-Sn(2)-O(15)	86.53(19)
F(6)-C(4)-F(5)	106.5(8)	O(9)-C(11)-H(11A)	109.6	O(11)#1-Sn(2)-O(15)#1	86.53(19)
O(5)-C(5)-C(6)	111.2(7)	O(9)-C(11)-H(11B)	109.6	O(11)-Sn(2)-O(15)#1	92.25(19)
O(6)-C(5)-O(5)	128.4(8)	O(9)-C(11)-C(12)	110.3(6)	O(13)-Sn(2)-O(11)	83.0(2)
O(6)-C(5)-C(6)	120.4(7)	H(11A)-C(11)-H(11B)	108.1	O(13)#1-Sn(2)-O(11)#1	83.0(2)
C(5)-O(5)-Sn(1)	124.5(5)	C(12)-C(11)-H(11A)	109.6	O(13)-Sn(2)-O(11)#1	175.03(19)

Table S12. Bond angles (in °) for compound **6**←(OEt$_2$)$_2$, *cont.*

O(13)#1-Sn(2)-O(11)	175.03(19)	H(22A)-C(22)-H(22B)	109.5	O(19)-C(27)-O(18)	127.0(7)
O(13)#1-Sn(2)-O(13)	96.8(3)	H(22A)-C(22)-H(22C)	109.5	O(19)-C(27)-C(28)	123.8(7)
O(13)#1-Sn(2)-O(15)#1	92.72(19)	H(22B)-C(22)-H(22C)	109.5	F(22)-C(28)-F(24)	105.7(7)
O(13)#1-Sn(2)-O(15)	88.51(19)	O(15)-C(23)-H(23A)	109.3	F(22)-C(28)-C(27)	109.7(7)
O(13)-Sn(2)-O(15)#1	88.51(19)	O(15)-C(23)-H(23B)	109.3	F(23)-C(28)-F(22)	108.0(8)
O(13)-Sn(2)-O(15)	92.71(19)	O(15)-C(23)-C(24)	111.6(7)	F(23)-C(28)-F(24)	109.0(8)
O(15)-Sn(2)-O(15)#1	178.2(3)	H(23A)-C(23)-H(23B)	108	F(23)-C(28)-C(27)	113.4(7)
C(17)-O(11)-Sn(2)	128.1(5)	C(24)-C(23)-H(23A)	109.3	F(24)-C(28)-C(27)	110.6(7)
C(19)-O(13)-Sn(2)	125.6(5)	C(24)-C(23)-H(23B)	109.3	O(20)-C(29)-H(29A)	109.4
C(21)-O(15)-Sn(2)	123.7(4)	C(23)-C(24)-H(24A)	109.5	O(20)-C(29)-H(29B)	109.4
C(23)-O(15)-Sn(2)	123.6(4)	C(23)-C(24)-H(24B)	109.5	O(20)-C(29)-C(30)	111.0(6)
C(23)-O(15)-C(21)	112.8(6)	C(23)-C(24)-H(24C)	109.5	H(29A)-C(29)-H(29B)	108
O(11)-C(17)-C(18)	109.5(7)	H(24A)-C(24)-H(24B)	109.5	C(30)-C(29)-H(29A)	109.4
O(12)-C(17)-O(11)	128.9(8)	H(24A)-C(24)-H(24C)	109.5	C(30)-C(29)-H(29B)	109.4
O(12)-C(17)-C(18)	121.6(8)	H(24B)-C(24)-H(24C)	109.5	C(29)-C(30)-H(30A)	109.5
F(13)-C(18)-F(14)	107.0(7)	O(16)#2-Sn(3)-O(16)	97.0(3)	C(29)-C(30)-H(30B)	109.5
F(13)-C(18)-C(17)	110.5(7)	O(16)#2-Sn(3)-O(18)#2	178.03(19)	C(29)-C(30)-H(30C)	109.5
F(14)-C(18)-C(17)	110.1(7)	O(16)#2-Sn(3)-O(18)	83.3(2)	H(30A)-C(30)-H(30B)	109.5
F(15)-C(18)-F(13)	107.9(7)	O(16)-Sn(3)-O(18)#2	83.3(2)	H(30A)-C(30)-H(30C)	109.5
F(15)-C(18)-F(14)	107.8(7)	O(16)-Sn(3)-O(18)	178.03(19)	H(30B)-C(30)-H(30C)	109.5
F(15)-C(18)-C(17)	113.3(7)	O(16)-Sn(3)-O(20)	90.64(19)	O(20)-C(31)-H(31A)	109.1
O(13)-C(19)-C(20)	110.8(7)	O(16)-Sn(3)-O(20)#2	88.49(19)	O(20)-C(31)-H(31B)	109.1
O(14)-C(19)-O(13)	128.5(8)	O(16)#2-Sn(3)-O(20)#2	90.64(19)	O(20)-C(31)-C(32)	112.5(6)
O(14)-C(19)-C(20)	120.7(7)	O(16)#2-Sn(3)-O(20)	88.49(19)	H(31A)-C(31)-H(31B)	107.8
F(16)-C(20)-F(17)	105.9(7)	O(18)#2-Sn(3)-O(18)	96.4(3)	C(32)-C(31)-H(31A)	109.1
F(16)-C(20)-F(18)	106.3(7)	O(18)#2-Sn(3)-O(20)	89.56(19)	C(32)-C(31)-H(31B)	109.1
F(16)-C(20)-C(19)	112.2(7)	O(18)-Sn(3)-O(20)	91.31(19)	C(31)-C(32)-H(32A)	109.5
F(17)-C(20)-F(18)	107.6(7)	O(18)#2-Sn(3)-O(20)#2	91.31(19)	C(31)-C(32)-H(32B)	109.5
F(17)-C(20)-C(19)	113.0(7)	O(18)-Sn(3)-O(20)#2	89.56(18)	C(31)-C(32)-H(32C)	109.5
F(18)-C(20)-C(19)	111.4(7)	O(20)-Sn(3)-O(20)#2	178.7(3)	H(32A)-C(32)-H(32B)	109.5
O(15)-C(21)-H(21A)	109.6	C(25)-O(16)-Sn(3)	126.5(5)	H(32A)-C(32)-H(32C)	109.5
O(15)-C(21)-H(21B)	109.6	C(27)-O(18)-Sn(3)	125.7(5)	H(32B)-C(32)-H(32C)	109.5
O(15)-C(21)-C(22)	110.4(6)	C(29)-O(20)-Sn(3)	124.6(4)	F(19)-C(26)-C(25)	106.0(9)
H(21A)-C(21)-H(21B)	108.1	C(29)-O(20)-C(31)	112.1(5)	F(20)-C(26)-F(19)	102.7(10)
C(22)-C(21)-H(21A)	109.6	C(31)-O(20)-Sn(3)	123.2(4)	F(20)-C(26)-F(21)	114.1(9)
C(22)-C(21)-H(21B)	109.6	O(16)-C(25)-C(26)	110.5(7)	F(20)-C(26)-C(25)	117.6(8)
C(21)-C(22)-H(22A)	109.5	O(17)-C(25)-O(16)	127.6(8)	F(21)-C(26)-F(19)	99.6(8)
C(21)-C(22)-H(22B)	109.5	O(17)-C(25)-C(26)	121.9(8)	F(21)-C(26)-C(25)	114.0(9)
C(21)-C(22)-H(22C)	109.5	O(18)-C(27)-C(28)	109.1(7)		

Symmetry transformations used to generate equivalent atoms: #1 ($-x$, y, $-z + 3/2$); #2 ($-x + 1$, y, $-z + 3/2$).

Crystallography of tetratin(II) monotin(IV) di-μ_3-oxy-octakis-μ-trifluoroacetate (**4**)

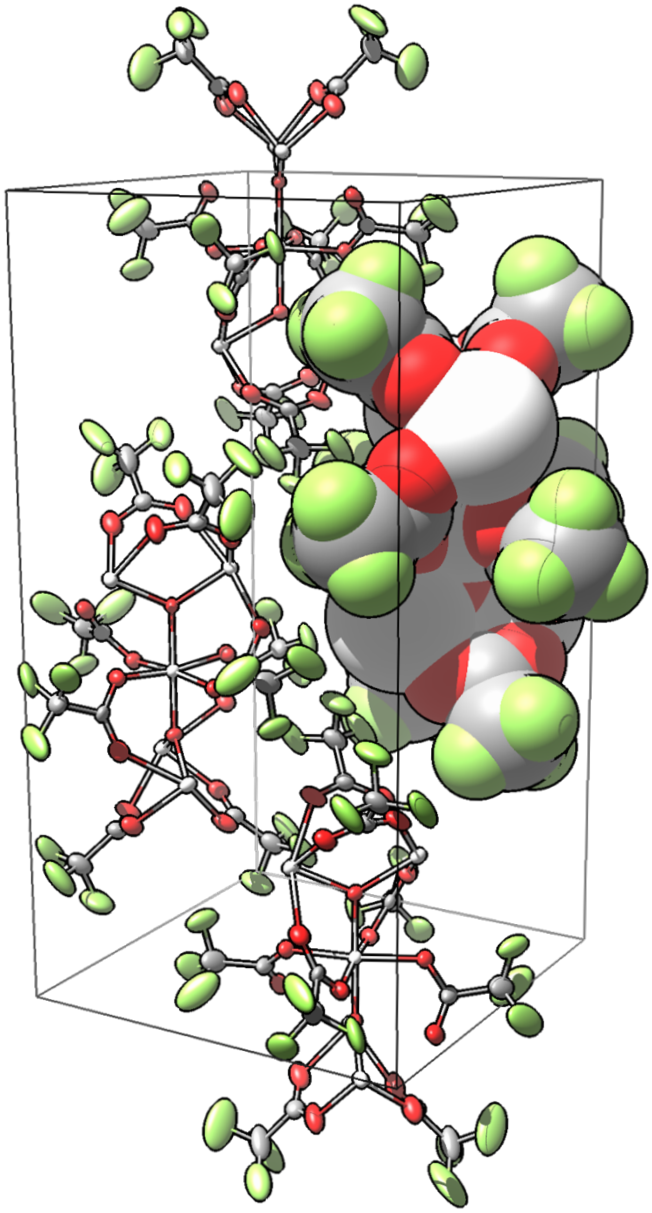

Figure S13. Crystal packing of **4**. Atoms are depicted as ellipsoids at 50% probability. One molecule of **3** is depicted as spacefilling spheres. The exposed Sn atoms (white) clearly show the location of the stereochemically active nonbonding lone-pairs.

Table S13. Selected crystallographic parameters for **4**.

Tetratin(II) monotin(IV) di-μ_3-oxy-octakis-μ-trifluoroacetate (**4**)	
Identification code	CCDC 1885256
Empirical formula	$C_{16}F_{24}O_{18}Sn_5$
Formula weight / g mol^{-1}	382.40
Temperature / K	125(2)
Wavelength / Å	0.71073
Crystal system	Orthorhombic
Space group	Pnna
Unit cell dimensions	a = 24.311(4) Å α = 90°
	b = 12.604(2) Å β = 90°
	c = 12.593(2) Å γ = 90°
Volume / Å^3	3858.5(11)
Z	4
ρ_{calc} / g cm^{-3}	2.633
μ / mm^{-1}	3.375
F(000)	2824
Crystal size / mm^3	0.20 × 0.12 × 0.12
θ range for data collection	1.675 to 26.999°.
Index ranges	$-31 \le h \le 28$
	$-16 \le k \le 16$
	$-16 \le l \le 16$
Reflections collected	40 644
Independent reflections	4218 [R(int) = 0.0778]
Completeness to θ = 26.000°	100.0 %
Absorption correction	Full-matrix least-squares on F^2
Max. and min. transmission	0.7458 and 0.6068
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4218 / 0 / 286
Goodness-of-fit on F^2	1.047
Final R indices [I > 2σ (I)]	R1 = 0.0392, ωR2 = 0.0918
R indices (all data)	R1 = 0.0547, ωR2 = 0.0988
Extinction coefficient	N/A
Largest diff. peak and hole / e Å^{-3}	2.002 and –1.313

Table S14. Bond lengths (in Å) for compound **4**.

Sn(1)-O(1)	2.008(5)	F(9)-C(6)	1.345(10)
Sn(1)-O(2)	2.011(5)	F(10)-C(8)	1.332(12)
Sn(1)-O(5)	2.077(4)	F(11)-C(8)	1.312(9)
Sn(1)-O(5)#1	2.077(4)	F(12)-C(8)	1.298(11)
Sn(1)-O(3)	2.080(4)	O(1)-Sn(2)#1	2.148(2)
Sn(1)-O(3)#1	2.080(4)	O(2)-Sn(3)#1	2.138(3)
Sn(2)-O(1)	2.148(2)	O(3)-C(1)	1.302(7)
Sn(2)-O(7)	2.177(4)	O(4)-C(1)	1.214(8)
Sn(2)-O(8)#1	2.317(4)	O(5)-C(3)	1.291(7)
Sn(2)-O(6)#1	2.436(4)	O(6)-C(3)	1.198(7)
Sn(3)-O(2)	2.138(3)	O(6)-Sn(2)#1	2.436(4)
Sn(3)-O(9)	2.166(5)	O(7)-C(5)	1.253(8)
Sn(3)-O(10)#1	2.319(5)	O(8)-C(5)	1.231(8)
Sn(3)-O(4)	2.551(5)	O(8)-Sn(2)#1	2.317(4)
F(1)-C(2)	1.324(11)	O(9)-C(7)	1.235(8)
F(2)-C(2)	1.269(9)	O(10)-C(7)	1.232(8)
F(3)-C(2)	1.314(9)	O(10)-Sn(3)#1	2.319(5)
F(4)-C(4)	1.332(8)	C(1)-C(2)	1.535(10)
F(5)-C(4)	1.307(9)	C(3)-C(4)	1.527(9)
F(6)-C(4)	1.313(8)	C(5)-C(6)	1.520(9)
F(7)-C(6)	1.289(9)	C(7)-C(8)	1.533(10)
F(8)-C(6)	1.314(9)		

Symmetry transformations used to generate equivalent atoms: #1 (x, $-y + {}^{1}/_{2}$, $-z + {}^{3}/_{2}$)

Table S15. Bond angles (in °) for compound **4**.

O(1)-Sn(1)-O(2)	180	C(7)-O(9)-Sn(3)	131.1(5)
O(1)-Sn(1)-O(5)	94.45(11)	C(7)-O(10)-Sn(3)#1	136.9(4)
O(2)-Sn(1)-O(5)	85.55(11)	O(4)-C(1)-O(3)	127.7(6)
O(1)-Sn(1)-O(5)#1	94.45(11)	O(4)-C(1)-C(2)	119.4(6)
O(2)-Sn(1)-O(5)#1	85.55(11)	O(3)-C(1)-C(2)	112.9(6)
O(5)-Sn(1)-O(5)#1	171.1(2)	F(2)-C(2)-F(3)	109.1(8)
O(1)-Sn(1)-O(3)	87.09(11)	F(2)-C(2)-F(1)	107.8(8)
O(2)-Sn(1)-O(3)	92.91(11)	F(3)-C(2)-F(1)	107.1(8)
O(5)-Sn(1)-O(3)	92.06(17)	F(2)-C(2)-C(1)	112.0(7)
O(5)#1-Sn(1)-O(3)	88.39(17)	F(3)-C(2)-C(1)	111.6(6)
O(1)-Sn(1)-O(3)#1	87.09(11)	F(1)-C(2)-C(1)	109.1(7)
O(2)-Sn(1)-O(3)#1	92.91(11)	O(6)-C(3)-O(5)	128.6(6)
O(5)-Sn(1)-O(3)#1	88.39(17)	O(6)-C(3)-C(4)	119.6(6)
O(5)#1-Sn(1)-O(3)#1	92.06(17)	O(5)-C(3)-C(4)	111.8(5)
O(3)-Sn(1)-O(3)#1	174.2(2)	F(5)-C(4)-F(6)	108.4(7)
O(1)-Sn(2)-O(7)	91.25(15)	F(5)-C(4)-F(4)	105.9(6)
O(1)-Sn(2)-O(8)#1	86.62(15)	F(6)-C(4)-F(4)	108.2(6)
O(7)-Sn(2)-O(8)#1	82.23(18)	F(5)-C(4)-C(3)	111.2(6)
O(1)-Sn(2)-O(6)#1	81.00(12)	F(6)-C(4)-C(3)	112.3(6)
O(7)-Sn(2)-O(6)#1	74.06(17)	F(4)-C(4)-C(3)	110.7(6)
O(8)#1-Sn(2)-O(6)#1	152.87(17)	O(8)-C(5)-O(7)	128.8(6)
O(2)-Sn(3)-O(9)	91.23(16)	O(8)-C(5)-C(6)	115.6(6)
O(2)-Sn(3)-O(10)#1	87.66(16)	O(7)-C(5)-C(6)	115.6(6)
O(9)-Sn(3)-O(10)#1	81.2(2)	F(7)-C(6)-F(8)	111.1(7)
O(2)-Sn(3)-O(4)	77.41(12)	F(7)-C(6)-F(9)	103.6(7)
O(9)-Sn(3)-O(4)	73.99(19)	F(8)-C(6)-F(9)	103.6(7)
O(10)#1-Sn(3)-O(4)	150.57(19)	F(7)-C(6)-C(5)	115.7(6)
Sn(1)-O(1)-Sn(2)	117.19(13)	F(8)-C(6)-C(5)	112.6(6)
Sn(1)-O(1)-Sn(2)#1	117.19(13)	F(9)-C(6)-C(5)	109.2(7)
Sn(2)-O(1)-Sn(2)#1	125.6(3)	O(10)-C(7)-O(9)	129.4(6)
Sn(1)-O(2)-Sn(3)	117.51(13)	O(10)-C(7)-C(8)	117.3(6)
Sn(1)-O(2)-Sn(3)#1	117.51(13)	O(9)-C(7)-C(8)	113.3(6)
Sn(3)-O(2)-Sn(3)#1	125.0(3)	F(12)-C(8)-F(11)	110.2(8)
C(1)-O(3)-Sn(1)	125.6(4)	F(12)-C(8)-F(10)	105.2(8)
C(1)-O(4)-Sn(3)	135.4(4)	F(11)-C(8)-F(10)	106.0(8)
C(3)-O(5)-Sn(1)	129.5(4)	F(12)-C(8)-C(7)	112.0(8)
C(3)-O(6)-Sn(2)#1	134.8(4)	F(11)-C(8)-C(7)	113.7(6)
C(5)-O(7)-Sn(2)	131.0(4)	F(10)-C(8)-C(7)	109.1(8)
C(5)-O(8)-Sn(2)#1	138.0(4)		

Symmetry transformations used to generate equivalent atoms: #1 (x, $-y + {}^{1}/_{2}$, $-z + {}^{3}/_{2}$)

Table S16. Torsion angles (in °) for compound **4**.

Sn(3)-O(4)-C(1)-O(3)	23.0(12)	Sn(2)#1-O(8)-C(5)-O(7)	-22.5(12)
Sn(3)-O(4)-C(1)-C(2)	-155.0(6)	Sn(2)#1-O(8)-C(5)-C(6)	158.4(5)
Sn(1)-O(3)-C(1)-O(4)	-8.2(11)	Sn(2)-O(7)-C(5)-O(8)	-4.1(11)
Sn(1)-O(3)-C(1)-C(2)	169.9(5)	Sn(2)-O(7)-C(5)-C(6)	174.9(5)
O(4)-C(1)-C(2)-F(2)	-15.0(12)	O(8)-C(5)-C(6)-F(7)	-165.2(7)
O(3)-C(1)-C(2)-F(2)	166.7(8)	O(7)-C(5)-C(6)-F(7)	15.6(10)
O(4)-C(1)-C(2)-F(3)	-137.6(7)	O(8)-C(5)-C(6)-F(8)	-36.0(10)
O(3)-C(1)-C(2)-F(3)	44.0(10)	O(7)-C(5)-C(6)-F(8)	144.9(7)
O(4)-C(1)-C(2)-F(1)	104.2(9)	O(8)-C(5)-C(6)-F(9)	78.5(8)
O(3)-C(1)-C(2)-F(1)	-74.1(8)	O(7)-C(5)-C(6)-F(9)	-100.7(8)
Sn(2)#1-O(6)-C(3)-O(5)	2.4(10)	Sn(3)#1-O(10)-C(7)-O(9)	14.2(13)
Sn(2)#1-O(6)-C(3)-C(4)	-176.0(4)	Sn(3)#1-O(10)-C(7)-C(8)	-166.3(6)
Sn(1)-O(5)-C(3)-O(6)	0.8(9)	Sn(3)-O(9)-C(7)-O(10)	13.5(12)
Sn(1)-O(5)-C(3)-C(4)	179.4(4)	Sn(3)-O(9)-C(7)-C(8)	-166.0(6)
O(6)-C(3)-C(4)-F(5)	105.7(7)	O(10)-C(7)-C(8)-F(12)	-133.1(8)
O(5)-C(3)-C(4)-F(5)	-72.9(7)	O(9)-C(7)-C(8)-F(12)	46.4(11)
O(6)-C(3)-C(4)-F(6)	-15.9(9)	O(10)-C(7)-C(8)-F(11)	-7.3(12)
O(5)-C(3)-C(4)-F(6)	165.4(6)	O(9)-C(7)-C(8)-F(11)	172.3(8)
O(6)-C(3)-C(4)-F(4)	-136.9(6)	O(10)-C(7)-C(8)-F(10)	110.8(8)
O(5)-C(3)-C(4)-F(4)	44.5(7)	O(9)-C(7)-C(8)-F(10)	-69.6(9)

Density Functional Theory (DFT) and Gas-Phase Electron Diffraction (GED) of 1 and 2

Table S17. Summary of experimental parameters relating to GED data collection for **1** and **2**.

Dataset Type	Short	Long
Nozzle-to-Image-Plate Distance / mm	234.5	477.0
Electron Wavelength / pm	5.85	5.85
$T_{\text{nozzle, av}}$ / K	473	473
$T_{\text{sample, av}}$ / K	463	463
Exposure Time / s	240	120

Table S18. Optimised Cartesian coordinates in Ångström (Å) and energy, E_{M06}, in atomic units (a.u) of **1** as calculated at the M06/def2-SVP level.

E_{M06} = -1265.69317741			
Sn	0.000000	0.000000	1.707022
O	-1.048348	1.833640	0.550225
O	0.994199	1.171554	0.069931
C	0.000000	1.933400	-0.103957
C	0.162487	3.028972	-1.168130
F	0.483841	2.481460	-2.329279
F	-0.944249	3.728492	-1.315563
F	1.140013	3.847870	-0.800076
O	-0.994199	-1.171554	0.069931
O	1.048348	-1.833640	0.550225
C	0.000000	-1.933400	-0.103957
C	-0.162487	-3.028972	-1.168130
F	-0.483841	-2.481460	-2.329279
F	0.944249	-3.728492	-1.315563
F	-1.140013	-3.847870	-0.800076

Table S19. Optimised Cartesian coordinates in Ångström (Å) and energy, E_{M06}, in atomic units (a.u) of **1** as calculated at the M06/def2-TZVP level.

E_{M06} = -1266.92692674			
Sn	0.000000	0.000000	1.661333
O	-1.060324	1.813728	0.520094
O	0.994300	1.173759	0.070970
C	0.000000	1.932403	-0.104085
C	0.179608	3.063751	-1.136388
F	0.596088	2.566562	-2.288579
F	-0.944081	3.718808	-1.335749
F	1.094638	3.915121	-0.688893
O	-0.994300	-1.173759	0.070970
O	1.060324	-1.813728	0.520094
C	0.000000	-1.932403	-0.104085
C	-0.179608	-3.063751	-1.136388
F	-0.596088	-2.566562	-2.288579
F	0.944081	-3.718808	-1.335749
F	-1.094638	-3.915121	-0.688893

Table S20. Optimised Cartesian coordinates in Ångström (Å) and energy, E_{M06}, in atomic units (a.u) of **1** as calculated at the M06/def2-QZVP level.

E_{M06} = -1266.98481147			
Sn	0.000000	0.000000	1.658676
O	-1.060599	1.812114	0.519136
O	0.993944	1.176451	0.073356
C	0.000000	1.934108	-0.101899
C	0.180116	3.066113	-1.134313
F	0.566287	2.563310	-2.294479
F	-0.935321	3.740119	-1.311906
F	1.117516	3.900630	-0.703567
O	-0.993944	-1.176451	0.073356
O	1.060599	-1.812114	0.519136
C	0.000000	-1.934108	-0.101899
C	-0.180116	-3.066113	-1.134313
F	-0.566287	-2.563310	-2.294479
F	0.935321	-3.740119	-1.311906
F	-1.117516	-3.900630	-0.703567

Table S21. Optimised Cartesian coordinates in Ångström (Å) and energy, E_{M11}, in atomic units (a.u) of **1** as calculated at the M11/def2-SVP level.

E_{M11} = -1265.50275815			
Sn	0.000000	0.000000	1.730656
O	-1.039459	1.797096	0.574018
O	0.986139	1.110571	0.103145
C	0.000000	1.881504	-0.093230
C	0.157241	2.948860	-1.193475
F	0.454398	2.360371	-2.350230
F	-0.956721	3.652911	-1.336402
F	1.153452	3.774124	-0.864866
O	-0.986139	-1.110571	0.103145
O	1.039459	-1.797096	0.574018
C	0.000000	-1.881504	-0.093230
C	-0.157241	-2.948860	-1.193475
F	-0.454398	-2.360371	-2.350230
F	0.956721	-3.652911	-1.336402
F	-1.153452	-3.774124	-0.864866

Table S22. Optimised Cartesian coordinates in Ångström (Å) and energy, E_{M11}, in atomic units (a.u) of **1** as calculated at the M11/def2-TZVP level.

E_{M11} = -1266.86015422			
Sn	0.000000	0.000000	1.691177
O	-1.050585	1.790073	0.550767
O	0.987683	1.118323	0.100031
C	0.000000	1.887197	-0.092651
C	0.172007	2.986154	-1.164197
F	0.577216	2.444564	-2.315643
F	-0.966841	3.639770	-1.369372
F	1.102798	3.859259	-0.753286
O	-0.987683	-1.118323	0.100031
O	1.050585	-1.790073	0.550767
C	0.000000	-1.887197	-0.092651
C	-0.172007	-2.986154	-1.164197
F	-0.577216	-2.444564	-2.315643
F	0.966841	-3.639770	-1.369372
F	-1.102798	-3.859259	-0.753286

Table S23. Optimised Cartesian coordinates in Ångström (Å) and energy, E_{M11}, in atomic units (a.u) of **1** as calculated at the M11/def2-QZVP level.

E_{M11} = -1266.95488084			
Sn	0.000000	0.000000	1.682033
O	-1.051903	1.785698	0.548154
O	0.989295	1.124835	0.099004
C	0.000000	1.890962	-0.091531
C	0.169495	2.996352	-1.157457
F	0.555814	2.457914	-2.316783
F	-0.965383	3.660999	-1.345375
F	1.112537	3.858338	-0.752750
O	-0.989295	-1.124835	0.099004
O	1.051903	-1.785698	0.548154
C	0.000000	-1.890962	-0.091531
C	-0.169495	-2.996352	-1.157457
F	-0.555814	-2.457914	-2.316783
F	0.965383	-3.660999	-1.345375
F	-1.112537	-3.858338	-0.752750

Table S24. Optimised Cartesian coordinates in Ångström (Å) and energy, $E_{SOGGA11X}$, in atomic units (a.u) of **1** as calculated at the SOGGA11X/def2-SVP level.

$E_{SOGGA11X}$ = -1265.63534406			
Sn	0.000000	0.000000	1.685318
O	-1.051982	1.830643	0.536282
O	0.989796	1.178947	0.073337
C	0.000000	1.945485	-0.106251
C	0.162344	3.063504	-1.152672
F	0.529757	2.546991	-2.316789
F	-0.964340	3.731107	-1.318873
F	1.103417	3.911126	-0.748380
O	-0.989796	-1.178947	0.073337
O	1.051982	-1.830643	0.536282
C	0.000000	-1.945485	-0.106251
C	-0.162344	-3.063504	-1.152672
F	-0.529757	-2.546991	-2.316789
F	0.964340	-3.731107	-1.318873
F	-1.103417	-3.911126	-0.748380

Table S25. Optimised Cartesian coordinates in Ångström (Å) and energy, $E_{SOGGA11X}$, in atomic units (a.u) of **1** as calculated at the SOGGA11X/def2-TZVP level.

$E_{SOGGA11X}$ = -1266.92648297			
Sn	0.000000	0.000000	1.619275
O	-1.066852	1.801994	0.497060
O	0.992210	1.182456	0.063369
C	0.000000	1.947460	-0.112335
C	0.181549	3.118114	-1.105911
F	0.719858	2.687882	-2.239003
F	-0.972267	3.701356	-1.378021
F	0.997322	4.023518	-0.566955
O	-0.992210	-1.182456	0.063369
O	1.066852	-1.801994	0.497060
C	0.000000	-1.947460	-0.112335
C	-0.181549	-3.118114	-1.105911
F	-0.719858	-2.687882	-2.239003
F	0.972267	-3.701356	-1.378021
F	-0.997322	-4.023518	-0.566955

Table S26. Optimised Cartesian coordinates in Ångström (Å) and energy, $E_{SOGGA11X}$, in atomic units (a.u) of **1** as calculated at the SOGGA11X/def2-QZVP level.

$E_{SOGGA11X}$ = -1266.97630535			
Sn	0.000000	0.000000	1.613998
O	-1.067231	1.799428	0.492956
O	0.992153	1.184646	0.061787
C	0.000000	1.948465	-0.113504
C	0.181888	3.123756	-1.101960
F	0.729995	2.701162	-2.232331
F	-0.972538	3.701480	-1.379468
F	0.988756	4.031128	-0.554325
O	-0.992153	-1.184646	0.061787
O	1.067231	-1.799428	0.492956
C	0.000000	-1.948465	-0.113504
C	-0.181888	-3.123756	-1.101960
F	-0.729995	-2.701162	-2.232331
F	0.972538	-3.701480	-1.379468
F	-0.988756	-4.031128	-0.554325

Table S27. Optimised Cartesian coordinates in Ångström (Å) and energy, $E_{SOGGA11\text{-}X}$, in atomic units (a.u) of **1** as calculated at the SOGGA11-X/DZP-DKH level.

$E_{SOGGA11\text{-}X}$ = -7223.11576523			
Sn	0.000000	0.000000	1.612842
O	-1.061598	1.837223	0.536052
C	0.000000	1.948392	-0.096176
O	0.979443	1.154423	0.076050
C	0.202365	3.090504	-1.109792
F	0.715135	2.624170	-2.244697
F	-0.939785	3.705880	-1.378547
F	1.055134	3.983672	-0.596984
O	1.061598	-1.837223	0.536052
C	0.000000	-1.948392	-0.096176
O	-0.979443	-1.154423	0.076050
C	-0.202365	-3.090504	-1.109792
F	-0.715135	-2.624170	-2.244697
F	0.939785	-3.705880	-1.378547
F	-1.055134	-3.983672	-0.596984

Table S28. Optimised Cartesian coordinates in Ångström (Å) and energy, $E_{SOGGA11\text{-}X}$, in atomic units (a.u) of **1** as calculated at the SOGGA11-X/TZP-DKH level.

$E_{SOGGA11\text{-}X}$ = -7223.43971935			
Sn	0.000000	0.000000	1.598760
O	-1.059238	1.815292	0.523365
C	0.000000	1.934374	-0.098943
O	0.977729	1.144936	0.069327
C	0.201989	3.092065	-1.099263
F	0.717390	2.642015	-2.234462
F	-0.939290	3.701919	-1.361764
F	1.045340	3.978358	-0.572807
O	1.059238	-1.815292	0.523365
C	0.000000	-1.934374	-0.098943
O	-0.977729	-1.144936	0.069327
C	-0.201989	-3.092065	-1.099263
F	-0.717390	-2.642015	-2.234462
F	0.939290	-3.701919	-1.361764
F	-1.045340	-3.978358	-0.572807

Table S29. Optimised Cartesian coordinates in Ångström (Å) and energy, E_{M06}, in atomic units (a.u) of **2** as calculated at the M06/def2-SVP level.

E_{M06} = -1555.31109592			
O	0.000000	0.000000	2.107330
Sn	1.456001	-1.055809	1.241794
Sn	-1.456001	1.055809	1.241794
O	0.000000	2.020142	-0.204815
C	1.072172	1.576845	-0.666501
O	1.643239	0.494192	-0.438086
C	1.784249	2.546835	-1.634150
F	2.269259	3.566818	-0.931037
F	2.782205	1.966446	-2.273252
F	0.929497	3.023039	-2.525925
O	0.000000	-2.020142	-0.204815
C	-1.072172	-1.576845	-0.666501
O	-1.643239	-0.494192	-0.438086
C	-1.784249	-2.546835	-1.634150
F	-2.269259	-3.566818	-0.931037
F	-2.782210	-1.966450	-2.273250
F	-0.929500	-3.023040	-2.525930

Table S30. Optimised Cartesian coordinates in Ångström (Å) and energy, E_{M06}, in atomic units (a.u) of **2** as calculated at the M06/def2-TZVP level.

E_{M06} = -1556.63610678			
O	0.000000	0.000000	2.065568
Sn	1.441379	1.038898	1.198573
Sn	-1.441379	-1.038898	1.198573
O	-1.708748	0.523912	-0.422447
C	-1.111917	1.588745	-0.663040
O	0.000000	1.981071	-0.273501
C	-1.908537	2.567575	-1.566448
F	-2.928100	3.057621	-0.866170
F	-1.168410	3.574546	-1.984139
F	-2.395079	1.935068	-2.621513
O	1.708748	-0.523912	-0.422447
C	1.111917	-1.588745	-0.663040
O	0.000000	-1.981071	-0.273501
C	1.908537	-2.567575	-1.566448
F	2.928100	-3.057621	-0.866170
F	1.168410	-3.574550	-1.984140
F	2.395079	-1.935070	-2.621510

Table S31. Optimised Cartesian coordinates in Ångström (Å) and energy, E_{M06}, in atomic units (a.u) of **2** as calculated at the M06/def2-QZVP level.

E_{M06} = -1556.70107571			
O	0.000000	0.000000	2.065354
Sn	1.441753	1.036272	1.204636
Sn	-1.441753	-1.036272	1.204636
O	-1.698962	0.521161	-0.419304
C	-1.106865	1.589086	-0.654413
O	0.000000	1.985759	-0.257964
C	-1.900154	2.556539	-1.573822
F	-2.998326	2.953226	-0.939082
F	-1.199097	3.622870	-1.899097
F	-2.263750	1.935220	-2.684671
O	1.698962	-0.521161	-0.419304
C	1.106865	-1.589086	-0.654413
O	0.000000	-1.985759	-0.257964
C	1.900154	-2.556539	-1.573822
F	2.998326	-2.953226	-0.939082
F	1.199097	-3.622870	-1.899100
F	2.263750	-1.935220	-2.684670

Table S32. Optimised Cartesian coordinates in Ångström (Å) and energy, E_{M11}, in atomic units (a.u) of **2** as calculated at the M11/def2-SVP level.

E_{M11} = -1554.89836428			
O	0.000000	0.000000	2.082411
Sn	1.442885	-1.083404	1.281121
Sn	-1.442885	1.083404	1.281121
O	0.000000	1.989831	-0.147188
C	1.048656	1.513593	-0.630176
O	1.602473	0.426799	-0.379092
C	1.721781	2.416895	-1.693911
F	1.963469	3.620683	-1.169738
F	2.866022	1.898073	-2.121743
F	0.899276	2.566247	-2.734181
O	0.000000	-1.989831	-0.147188
C	-1.048656	-1.513593	-0.630176
O	-1.602473	-0.426799	-0.379092
C	-1.721781	-2.416895	-1.693911
F	-1.963469	-3.620683	-1.169738
F	-2.866020	-1.898070	-2.121740
F	-0.899280	-2.566250	-2.734180

Table S33. Optimised Cartesian coordinates in Ångström (Å) and energy, E_{M11}, in atomic units (a.u) of **2** as calculated at the M11/def2-TZVP level.

E_{M11} = -1556.36439404			
O	0.000000	0.000000	2.051543
Sn	1.435490	-1.070803	1.242349
Sn	-1.435490	1.070803	1.242349
O	0.000000	1.988985	-0.176252
C	1.064815	1.533526	-0.636439
O	1.619600	0.446283	-0.404534
C	1.780518	2.486329	-1.635133
F	2.124945	3.617054	-1.000790
F	2.878928	1.934089	-2.144382
F	0.952982	2.802236	-2.637927
O	0.000000	-1.988985	-0.176252
C	-1.064815	-1.533526	-0.636439
O	-1.619600	-0.446283	-0.404534
C	-1.780518	-2.486329	-1.635133
F	-2.124945	-3.617054	-1.000790
F	-2.878930	-1.934090	-2.144380
F	-0.952980	-2.802240	-2.637930

Table S34. Optimised Cartesian coordinates in Ångström (Å) and energy, E_{M11}, in atomic units (a.u) of **2** as calculated at the M11/def2-QZVP level.

E_{M11} = -1556.46771071			
O	0.000000	0.000000	2.047599
Sn	1.431937	-1.065305	1.233184
Sn	-1.431937	1.065305	1.233184
O	0.000000	1.985434	-0.183310
C	1.071132	1.538144	-0.635319
O	1.629238	0.452915	-0.403951
C	1.791777	2.500086	-1.622376
F	2.127229	3.627455	-0.977846
F	2.895774	1.955538	-2.126659
F	0.971299	2.819675	-2.629423
O	0.000000	-1.985434	-0.183310
C	-1.071132	-1.538144	-0.635319
O	-1.629238	-0.452915	-0.403951
C	-1.791777	-2.500086	-1.622376
F	-2.127229	-3.627455	-0.977846
F	-2.895770	-1.955540	-2.126660
F	-0.971300	-2.819680	-2.629420

Table S35. Optimised Cartesian coordinates in Ångström (Å) and energy, $E_{SOGGA11X}$, in atomic units (a.u) of **2** as calculated at the SOGGA11Z/def2-SVP level.

	$E_{SOGGA11X}$ =	-1555.22139679	
O	0.000000	0.000000	2.041502
Sn	1.449558	-1.070045	1.203839
Sn	-1.449558	1.070045	1.203839
O	0.000000	1.900274	-0.331632
C	1.153369	1.564599	-0.664230
O	1.803687	0.550473	-0.341757
C	1.905490	2.563047	-1.576095
F	2.650025	3.362606	-0.811325
F	2.705446	1.930255	-2.420635
F	1.066750	3.313707	-2.271252
O	0.000000	-1.900274	-0.331632
C	-1.153369	-1.564599	-0.664230
O	-1.803687	-0.550473	-0.341757
C	-1.905490	-2.563047	-1.576095
F	-2.650025	-3.362606	-0.811325
F	-2.705450	-1.930260	-2.420640
F	-1.066750	-3.313710	-2.271250

Table S36. Optimised Cartesian coordinates in Ångström (Å) and energy, $E_{SOGGA11X}$, in atomic units (a.u) of **2** as calculated at the SOGGA11Z/def2-TZVP level.

	$E_{SOGGA11X}$ =	-1556.61033066	
O	0.000000	0.000000	2.008527
Sn	1.429650	-1.052697	1.166550
Sn	-1.429650	1.052697	1.166550
O	0.000000	1.916035	-0.335373
C	1.152721	1.577421	-0.662338
O	1.785071	0.543167	-0.376837
C	1.933300	2.612284	-1.521664
F	2.636442	3.399635	-0.702699
F	2.777175	2.016022	-2.350913
F	1.115821	3.375218	-2.230823
O	0.000000	-1.916035	-0.335373
C	-1.152721	-1.577421	-0.662338
O	-1.785071	-0.543167	-0.376837
C	-1.933300	-2.612284	-1.521664
F	-2.636442	-3.399635	-0.702699
F	-2.777180	-2.016020	-2.350910
F	-1.115820	-3.375220	-2.230820

Table S37. Optimised Cartesian coordinates in Ångström (Å) and energy, $E_{SOGGA11X}$, in atomic units (a.u) of **2** as calculated at the SOGGA11Z/def2-QZVP level.

$E_{SOGGA11X}$ = -1556.66621870			
O	0.000000	0.000000	2.001673
Sn	1.428519	-1.052149	1.163798
Sn	-1.428519	1.052149	1.163798
O	0.000000	1.911985	-0.338232
C	1.154119	1.577071	-0.661498
O	1.787354	0.544621	-0.374294
C	1.935074	2.614485	-1.517644
F	2.633073	3.403139	-0.696435
F	2.782978	2.021157	-2.343737
F	1.118453	3.375155	-2.228887
O	0.000000	-1.911985	-0.338232
C	-1.154119	-1.577071	-0.661498
O	-1.787354	-0.544621	-0.374294
C	-1.935074	-2.614485	-1.517644
F	-2.633073	-3.403139	-0.696435
F	-2.782980	-2.021160	-2.343740
F	-1.118450	-3.375160	-2.228890

Table S38. Optimised Cartesian coordinates in Ångström (Å) and energy, $E_{SOGGA11\text{-}X}$, in atomic units (a.u) of **2** as calculated at the SOGGA11-X/DZP-DKH level.

$E_{SOGGA11\text{-}X}$ = -13468.42020240			
O	0.000000	0.000000	1.973834
Sn	-1.772424	0.093961	1.197833
Sn	1.772424	-0.093961	1.197833
O	-1.052677	1.552379	-0.316350
C	0.098920	1.917634	-0.643647
O	1.204998	1.440108	-0.308959
C	0.149879	3.159339	-1.569328
F	0.000000	4.261413	-0.821332
F	1.307780	3.249456	-2.212301
F	-0.830704	3.130947	-2.467109
O	1.052677	-1.552379	-0.316350
C	-0.098920	-1.917634	-0.643647
O	-1.204998	-1.440108	-0.308959
C	-0.149879	-3.159339	-1.569328
F	0.000000	-4.261413	-0.821332
F	-1.307780	-3.249456	-2.212301
F	0.830704	-3.130947	-2.467109

Table S39. Optimised Cartesian coordinates in Ångström (Å) and energy, $E_{SOGGA11\text{-}X}$, in atomic units (a.u) of **2** as calculated at the SOGGA11-X/TZP-DKH level.

$E_{SOGGA11\text{-}X}$ = -13468.92089320			
O	0.000000	0.000000	1.963780
Sn	-1.742033	0.194316	1.172353
Sn	1.742033	-0.194316	1.172353
O	-0.950360	1.616093	-0.343302
C	0.216810	1.936161	-0.636750
O	1.291301	1.401412	-0.312804
C	0.326057	3.203517	-1.529186
F	0.000000	4.275514	-0.805751
F	1.551374	3.374063	-1.995945
F	-0.509566	3.124521	-2.557005
O	0.950360	-1.616093	-0.343302
C	-0.216810	-1.936161	-0.636750
O	-1.291301	-1.401412	-0.312804
C	-0.326057	-3.203517	-1.529186
F	0.000000	-4.275514	-0.805751
F	-1.551374	-3.374063	-1.995945
F	0.509566	-3.124521	-2.557005

Table S40. Definitions of the parameters used in the parameterized molecular model of **1** and **2**.

	Parameter	Definition
p_1	rSn-O[a]	$^2/_5$ rSn(17)-O(16) + $^1/_5$ rSn(17)-O(19) + $^1/_5$ rSn(1)-O(2) + $^1/_5$ rSn(1)-O(4)
p_2	rSn-O[b]	{$^2/_3$ rSn(17)-O(16) + $^1/_3$ rSn(17)-O(19)} – {$^1/_2$ rSn(1)-O(2) + $^1/_2$ rSn(1)-O(4)}
p_3	rSn-O[b]	rSn(17)-O(16) – rSn(17)-O(19)
p_4	rSn-O[b]	rSn(1)-O(2) – rSn(1)-O(4)
p_5	rSn-C (**1**)	rSn(1)-C(3)
p_6	rSn-C (**2**)	rSn(17)-C(20)
p_7	rC-O[a]	$^1/_2$ rC(20)-O(19) + $^1/_4$ rC(3)-O(2) + $^1/_4$ rC(3)-O(4)
p_8	rC-O[b]	rC(20)-O(19) – {$^1/_2$ rC(3)-O(2) + $^1/_2$ rC(3)-O(4)}
p_9	rC-O[b]	rC(3)-O(4) – rC(3)-O(2)
p_{10}	rC-C[a]	$^1/_2$ rC(20)-C(22) + $^1/_2$ rC(3)-C(5)
p_{11}	rC-F[a]	$^1/_6$ {rC(5)-F(6) + rC(5)-F(7) + rC(5)-F(8) + rC(22)-F(23) + rC(22)-F(24) + rC(22)-F(25)}
p_{12}	aC-C-F[a]	$^1/_6$ {aC(3)-C(5)-F(6) + aC(3)-C(5)-F(7) + aC(3)-C(5)-F(8) + aC(20)-C(22)-F(23) + aC(20)-C(22)-F(24) + aC(20)-C(22)-F(25)}
p_{13}	aO-C-C (**1**)	aO(2)-C(3)-C(5)
p_{14}	aC-Sn-C (**1**)	aC(3)-Sn(1)-C(10)
p_{15}	øO-C-C-F (**1**)	øO(2)-C(3)-C(5)-F(6)
p_{16}	øO-C-C-F (**1**)	øO(2)-C(3)-C(5)-F(7)
p_{17}	øO-C-C-F (**1**)	øO(2)-C(3)-C(5)-F(8)
p_{18}	øX[c]-Sn-C-O (**1**)	øX[c]-Sn(1)-C(3)-O(2)
p_{19}	aSn-O-Sn (**2**)	aSn(17)-O(16)-Sn(18)
p_{20}	øO-C-C-F (**2**)	øO(19)-C(20)-C(22)-F(23)
p_{21}	øO-C-C-F (**2**)	øO(19)-C(20)-C(22)-F(24)
p_{22}	øO-C-C-F (**2**)	øO(19)-C(20)-C(22)-F(25)
p_{23}	aC-X[d]-C (**2**)	aC(20)-X[d]-C(27)

[a] Multiplicity-weighted average. [b] Refinable difference. [c] X lies on the principle symmetry axis of **1**. [d] X lies at the centroid of Sn(17) and Sn(18).

Table S41. Summary of experimental parameters relating to GED data reduction and refinement for **1** and **2**.

Dataset Type	Short	Long
Δs / nm^{-1}	2.0	1.0
s_{min} / nm^{-1}	88.0	50.0
sw_1 / nm^{-1}	104.0	68.0
sw_2 / nm^{-1}	222.0	101.0
s_{max} / nm^{-1}	240.0	114.0
Correlation Parameter	0.4934	0.4959
Scale Factor (k)	0.0049(1)	0.0022(1)

Table S42. Refined (r_{h1}) and theoretical[a] (r_e) parameter values[b] and SARACEN restraints[c] applied in the least-squares refinement of **1** and **2**.

	r_{h1}	r_e	Restraint
p_1	215.8(7)	217.6	–
p_2	−13.8(10)	−13.0	−13.0(7)
p_3	33.6(11)	30.1	30.1(18)
p_4	22.1(21)	21.5	21.5(18)
p_5	260.0(7)	257.4	–
p_6	317.2(7)	318.5	–
p_7	125.8(2)	124.8	–
p_8	−0.5(1)	−0.6	−0.6(1)
p_9	3.4(4)	3.4	3.4.(4)
p_{10}	153.1(6)	154.9	–
p_{11}	133.7(1)	132.7	–
p_{12}	110.7(1)	110.4	110.4(1)
p_{13}	120.8(3)	120.8	120.8(3)
p_{14}	97.5(3)	97.5	97.5(3)
p_{15}	−133.4[d]	−133.4	–
p_{16}	−12.4 [d]	−12.4	–
p_{17}	107.3 [d]	107.3	–
p_{18}	−69.8 [d]	−69.8	–
p_{19}	137.4(17)	131.4	131.4(17)
p_{20}	70.7 [d]	70.7	–
p_{21}	−169.5 [d]	−169.5	–
p_{22}	−48.3 [d]	−48.3	–
p_{23}	94.2(1)	94.2	–

[a] Calculations at the SOGGA11X/TZP-DKH level. [b] Interatomic distances (r) are tabulated in picometers (pm) and angles (a) are tabulated in degrees. [c] SARACEN restraint uncertainties are derived from sequential DFT geometry optimizations using the M06, M11 and SOGGA11X functionals and the def2-SVP, def2-TZVP and def2-QZVP basis sets. [d] Unrefined; no information available.

Table S43. Least-squares correlation matrix[a] (×100) of **1** and **2**.

	p_1	p_3	p_4	p_5	p_6	p_7	p_{10}	p_{11}	p_{19}	u_1	u_2	u_3	u_{13}	u_{42}	u_{65}	u_{74}	k_1	k_2
p_1	100						-60		-74		-51							
p_3		100							66									
p_4			100							-53		-78						
p_5				100			-52											
p_6					100						51							
p_7						100		-60						61				
p_{10}							100										50	55
p_{11}								100										
p_{19}									100		55							
u_1										100		69						
u_2											100		94					
u_3												100						
u_{13}													100			51		
u_{42}														100			65	
u_{65}															100	59		
u_{74}																100		
k_1																	100	
k_2																		100

[a] Only values ≥ 50% are tabulated. k_1 and k_2 are scale factors.

Table S44. Internuclear distances (r_a / pm), refined (u_{GED}) and theoretical (u_{h1}) amplitudes of vibration and restraints and distance corrections (k_{h1}) for **1** and **2**.[a]

Amp.	Atomic Pair	r_a	u_{GED}	Restraint	k_{h1}	u_{h1}
u_8	O(2)-C(3)	124.4(3)	2.9 (Tied to u_{42})	–	4.2	0.1
u_{93}	C(20)-O(21)	125.5(3)	2.8 (Tied to u_{42})	–	4.0	0.1
u_{80}	O(19)-C(20)	125.5(3)	2.8 (Tied to u_{42})	–	4.0	0.1
u_{21}	C(3)-O(4)	127.8(3)	2.8 (Tied to u_{42})	–	4.0	0.1
u_{42}	C(5)...F(7)	132.8(1)	3.8(1)	5.6(6)	5.6	0.1
u_{41}	C(5)...F(6)	133.4(1)	2.8 (Tied to u_{42})	–	4.1	0.1
u_{114}	C(22)...F(24)	133.6(1)	3.2 (Tied to u_{42})	–	4.7	0.1
u_{115}	C(22)...F(25)	133.8(1)	3.3 (Tied to u_{42})	–	4.7	0.1
u_{43}	C(5)...F(8)	134.0(1)	3.5 (Tied to u_{42})	–	5.1	0.1
u_{113}	C(22)...F(23)	134.8(1)	3.3 (Tied to u_{42})	–	4.8	0.1
u_{22}	C(3)-C(5)	152.6(6)	6.6(1)	5.1(5)	5.1	0.1
u_{94}	C(20)-C(22)	153.2(6)	6.6 (Tied to u_{22})	–	5.1	0.1
u_{57}	O(16)-Sn(17)	187.8(11)	5.5(1)	5.3(5)	5.3	0.1
u_9	O(2)...O(4)	210.6(11)	3.4 (Tied to u_3)	–	4.9	0.1
u_3	Sn(1)-O(4)	212.9(14)	9.5(6)	13.7(14)	13.7	0.4
u_{120}	F(23)...F(24)	215.6(3)	4.5 (Tied to u_3)	–	6.6	0.1
u_{48}	F(6)...F(7)	216.0(3)	9.0 (Tied to u_3)	–	13.0	0.3
u_{53}	F(7)...F(8)	216.2(3)	6.6 (Tied to u_3)	–	9.6	0.1
u_{49}	F(6)...F(8)	216.7(3)	5.6 (Tied to u_3)	–	8.1	0.1
u_{121}	F(23)...F(25)	217.2(3)	4.6 (Tied to u_3)	–	6.6	0.1
u_{125}	F(24)...F(25)	218.3(3)	4.4 (Tied to u_3)	–	6.4	0.1
u_{75}	Sn(17)...O(28)	221.4(9)	6.5 (Tied to u_3)	–	9.4	0.2
u_{66}	Sn(17)-O(19)	221.4(9)	6.5 (Tied to u_3)	–	9.3	0.2
u_{81}	O(19)...O(21)	229.0(13)	3.8 (Tied to u_3)	–	5.5	0.1
u_{25}	C(3)-F(8)	233.8(6)	15.0 (Tied to u_1)	–	24.2	0.6
u_{97}	C(20)-F(25)	233.8(6)	4.9 (Tied to u_1)	–	7.9	0.1
u_{104}	O(21)...C(22)	234.8(10)	4.4 (Tied to u_1)	–	7.1	0.1
u_{82}	O(19)...C(22)	234.8(10)	4.4 (Tied to u_1)	–	7.1	0.1
u_1	Sn(1)-O(2)	235.1(14)	5.6(5)	9.1(9)	9.1	0.2
u_{23}	C(3)-F(6)	235.3(6)	15.3 (Tied to u_1)	–	24.6	0.5
u_{24}	C(3)-F(7)	236.0(6)	12.6 (Tied to u_1)	–	20.4	0.3
u_{96}	C(20)-F(24)	238.1(6)	4.7 (Tied to u_1)	–	7.5	0.1
u_{95}	C(20)-F(23)	238.9(6)	5.4 (Tied to u_1)	–	8.8	0.2
u_{10}	O(2)...C(5)	241.5(7)	4.8 (Tied to u_1)	–	7.7	0.1
u_{32}	O(4)...C(5)	250.2(14)	4.6 (Tied to u_1)	–	7.5	0.1
u_{106}	O(21)...F(24)	255.3(13)	18.9 (Tied to u_2)	–	18.8	0.7
u_{85}	O(19)...F(25)	266.4(12)	21.1 (Tied to u_2)	–	21.0	0.8
u_2	Sn(1)...C(3)	267.1(7)	7.0(3)	–	7.0	0.1
u_{34}	O(4)...F(7)	274.5(20)	50.3 (Tied to u_2)	–	50.1	5.4

Table S44. Internuclear distances (r_a / pm), refined (u_{GED}) and theoretical (u_{h1}) amplitudes of vibration and restraints and distance corrections (k_{h1}) for **1** and **2**, *cont.*[a]

u_{11}	O(2)...F(6)	275.0(8)	52.5 (Tied to u_2)	–	52.3	4.9
u_{60}	O(16)...O(21)	287.7(28)	13.8 (Tied to u_{13})	–	15.1	0.4
u_{58}	O(16)...O(19)	287.7(28)	13.7 (Tied to u_{13})	–	15.0	0.4
u_{83}	O(19)...F(23)	289.0(11)	30.5 (Tied to u_{13})	–	33.4	1.9
u_{13}	O(2)...F(8)	289.1(7)	66.7(23)	–	72.9	8.5
u_{16}	O(2)...O(11)	302.6(16)	22.8 (Tied to u_{13})	–	24.9	1.0
u_{88}	O(19)...O(28)	312.1(15)	16.8 (Tied to u_{74})	–	22.4	0.8
u_{59}	O(16)...C(20)	314.9(23)	11.4 (Tied to u_{74})	–	15.3	0.4
u_{74}	Sn(17)...C(27)	317.2(7)	8.4(7)	11.2(11)	11.2	0.2
u_{67}	Sn(17)...C(20)	317.2(7)	8.1 (Tied to u_{74})	–	10.8	0.2
u_{105}	O(21)...F(23)	321.2(9)	25.9 (Tied to u_{74})	–	34.6	1.9
u_{33}	O(4)...F(6)	323.7(11)	95.3 (Tied to u_{65})	–	53.6	4.0
u_{35}	O(4)...F(8)	327.9(12)	56.9 (Tied to u_{74})	–	76.0	8.4
u_{14}	O(2)...O(9)	327.9(21)	45.2 (Tied to u_{65})	–	25.5	0.4
u_{107}	O(21)...F(25)	328.9(8)	32.9 (Tied to u_{65})	–	18.5	0.5
u_{15}	O(2)...C(10)	343.0(16)	45.6 (Tied to u_{65})	–	25.7	1.0
u_{86}	O(19)...O(26)	344.8(20)	105.1 (Tied to u_{65})	–	59.2	-13.8
u_{12}	O(2)...F(7)	345.8(6)	44.1 (Tied to u_{65})	–	24.8	0.9
u_{84}	O(19)...F(24)	347.1(7)	22.5 (Tied to u_{65})	–	12.7	0.3
u_{65}	Sn(17)...Sn(18)	348.6(5)	12.4(3)	7.0(7)	7.0	-1.0
u_{108}	O(21)...O(28)	352.3(19)	97.5 (Tied to u_{65})	–	54.9	-10.3
u_{73}	Sn(17)...O(26)	357.0(10)	32.3 (Tied to u_{65})	–	18.2	0.5
u_{68}	Sn(17)...O(21)	357.2(10)	30.4 (Tied to u_{65})	–	17.1	0.4
u_{87}	O(19)...C(27)	358.1(10)	72.0 (Tied to u_{65})	–	40.5	2.3
u_{99}	C(20)...O(28)	360.0(10)	65.6 (Tied to u_{65})	–	36.9	1.9
u_{36}	O(4)...O(11)	371.0(28)	37.6 (Tied to u_{65})	–	21.1	-3.5
u_{98}	C(20)...C(27)	374.3(11)	45.6 (Tied to u_{65})	–	25.6	-8.0
u_{27}	C(3)...O(11)	381.4(14)	39.6 (Tied to u_{65})	–	22.3	0.6
u_{26}	C(3)...C(10)	395.2(13)	41.8 (Tied to u_{65})	–	23.5	-2.1
u_4	Sn(1)...C(5)	419.8(7)	8.1(7)	–	8.3	0.1
u_{69}	Sn(17)...C(22)	453.0(9)	12.3 (Tied to u_{78})	–	14.0	0.2
u_{76}	Sn(17)...C(29)	453.0(9)	11.9 (Tied to u_{78})	–	13.5	0.2
u_{61}	O(16)...C(22)	466.8(21)	18.7 (Tied to u_{78})	–	21.2	0.5
u_{17}	O(2)...C(12)	470.9(12)	32.3 (Tied to u_{78})	–	36.5	1.5
u_{78}	Sn(17)...F(31)	471.0(9)	22.1(6)	–	24.9	0.6
u_{72}	Sn(17)...F(25)	478.9(9)	23.9 (Tied to u_{78})	–	27.0	0.8
u_7	Sn(1)...F(8)	481.2(6)	24.6 (Tied to u_{78})	–	27.8	0.5
u_6	Sn(1)...F(7)	481.3(12)	19.9 (Tied to u_{78})	–	22.5	0.4
u_5	Sn(1)...F(6)	485.2(6)	21.3 (Tied to u_{78})	–	24.0	0.4
u_{18}	O(2)...F(13)	487.1(13)	88.9 (Tied to u_{78})	–	100.4	10.5
u_{112}	O(21)...F(32)	489.2(10)	54.2 (Tied to u_{70})	–	56.3	3.1

Table S44. Internuclear distances (r_a / pm), refined (u_{GED}) and theoretical (u_{h1}) amplitudes of vibration and restraints and distance corrections (k_{h1}) for **1** and **2**, *cont.*.[a]

u_{89}	O(19)...C(29)	494.4(10)	45.3 (Tied to u_{70})	–	47.1	2.2
u_{109}	O(21)...C(29)	494.7(10)	41.7 (Tied to u_{70})	–	43.4	1.9
u_{70}	Sn(17)...F(23)	499.4(9)	38.4(55)	–	39.9	1.6
u_{19}	O(2)...F(14)	504.0(14)	75.5 (Tied to u_{70})	–	78.5	6.1
u_{100}	C(20)...C(29)	509.4(11)	38.2 (Tied to u_{77})	–	37.6	1.4
u_{103}	C(20)...F(32)	512.6(11)	60.6 (Tied to u_{77})	–	59.7	3.3
u_{91}	O(19)...F(31)	516.2(10)	57.9 (Tied to u_{77})	–	57.0	3.1
u_{62}	O(16)...F(23)	518.8(17)	41.6 (Tied to u_{77})	–	40.9	1.6
u_{37}	O(4)...C(12)	521.5(12)	29.8 (Tied to u_{77})	–	29.3	0.8
u_{29}	C(3)...F(13)	521.6(16)	91.0 (Tied to u_{77})	–	89.6	7.3
u_{92}	O(19)...F(32)	525.2(9)	68.0 (Tied to u_{77})	–	67.0	4.1
u_{28}	C(3)...C(12)	526.0(13)	36.3 (Tied to u_{77})	–	35.7	1.2
u_{77}	Sn(17)...F(30)	527.4(9)	40.2(21)	–	39.6	1.5
u_{38}	O(4)...F(13)	532.5(14)	63.0 (Tied to u_{77})	–	62.0	3.1
u_{63}	O(16)...F(24)	532.9(21)	24.6 (Tied to u_{77})	–	24.3	0.5
u_{64}	O(16)...F(25)	534.0(24)	21.4 (Tied to u_{77})	–	21.1	0.4
u_{79}	Sn(17)...F(32)	536.9(8)	20.2 (Tied to u_{77})	–	19.9	0.3
u_{128}	F(25)...F(32)	540.4(13)	111.5 (Tied to u_{77})	–	109.8	-10.2
u_{102}	C(20)...F(31)	549.6(11)	76.8 (Tied to u_{71})	–	57.6	2.9
u_{71}	Sn(17)...F(24)	554.0(8)	20.8(16)	15.6(16)	15.6	0.2
u_{111}	O(21)...F(31)	562.4(10)	81.4 (Tied to u_{71})	–	61.0	3.3
u_{20}	O(2)...F(15)	574.5(13)	60.9 (Tied to u_{71})	–	45.7	1.6
u_{30}	C(3)...F(14)	575.3(14)	103.2 (Tied to u_{71})	–	77.4	5.2
u_{119}	C(22)...F(32)	587.7(13)	83.2 (Tied to u_{127})	–	82.4	5.2
u_{116}	C(22)...C(29)	588.1(13)	56.6 (Tied to u_{127})	–	56.1	-19.2
u_{110}	O(21)...F(30)	589.0(10)	39.6 (Tied to u_{127})	–	39.2	1.3
u_{40}	O(4)...F(15)	591.7(13)	81.8 (Tied to u_{127})	–	81.1	5.6
u_{127}	F(24)...F(32)	593.7(14)	107.0(10)	–	106.1	8.7
u_{45}	C(5)...F(13)	597.2(20)	121.8 (Tied to u_{127})	–	120.7	11.3
u_{39}	O(4)...F(14)	600.0(14)	57.7 (Tied to u_{127})	–	57.2	2.6
u_{90}	O(19)...F(30)	604.7(10)	42.7 (Tied to u_{127})	–	42.3	1.5
u_{101}	C(20)...F(30)	619.9(11)	30.3 (Tied to u_{127})	–	30.1	0.7
u_{31}	C(3)...F(15)	620.7(13)	72.5 (Tied to u_{127})	–	71.8	4.0
u_{44}	C(5)...C(12)	622.1(16)	55.5 (Tied to u_{127})	–	55.0	-7.2
u_{50}	F(6)...F(13)	634.6(26)	176.6 (Tied to u_{127})	–	175.0	23.3
u_{51}	F(6)...F(14)	636.8(21)	164.0 (Tied to u_{127})	–	162.5	21.8
u_{118}	C(22)...F(31)	641.9(13)	81.4 (Tied to u_{127})	–	80.7	4.9
u_{126}	F(24)...F(31)	659.4(13)	106.0 (Tied to u_{127})	–	105.0	-23.3
u_{46}	C(5)...F(14)	683.5(16)	108.8 (Tied to u_{127})	–	107.8	8.6
u_{54}	F(7)...F(14)	697.0(16)	131.3 (Tied to u_{127})	–	130.1	-48.6
u_{52}	F(6)...F(15)	711.0(19)	143.0 (Tied to u_{127})	–	141.7	13.0

Table S44. Internuclear distances (r_a / pm), refined (u_{GED}) and theoretical (u_{h1}) amplitudes of vibration and restraints and distance corrections (k_{h1}) for **1** and **2**, *cont.*.[a]

u_{124}	F(23)...F(32)	719.9(13)	75.7 (Tied to u_{127})	–	75.0	3.7
u_{117}	C(22)...F(30)	731.0(13)	47.5 (Tied to u_{127})	–	47.1	1.4
u_{47}	C(5)...F(15)	732.3(15)	97.4 (Tied to u_{127})	–	96.6	5.9
u_{56}	F(8)...F(15)	736.2(14)	113.1 (Tied to u_{127})	–	112.1	-56.5
u_{123}	F(23)...F(31)	758.3(13)	74.3 (Tied to u_{127})	–	73.6	3.5
u_{55}	F(7)...F(15)	767.2(16)	159.2 (Tied to u_{127})	–	157.8	15.3
u_{122}	F(23)...F(30)	806.7(14)	36.2 (Tied to u_{127})	–	35.9	-42.5

[a] All values are tabulated in picometers (pm).

Table S45. Refined Cartesian coordinates in Ångström (Å) for the experimentally-determined structure of **1** obtained *via* GED.

	x	*y*	*z*
Sn	0.0000	0.0000	-1.6390
O	1.0391	-1.2922	0.0070
C	0.0287	-2.0100	0.1254
O	-0.9177	-1.6545	-0.6586
C	0.0049	-3.1802	1.1323
F	0.4790	-2.7953	2.3184
F	-1.2259	-3.6519	1.3021
F	0.7773	-4.1750	0.6732
O	-1.0391	1.2922	0.0070
C	-0.0287	2.0100	0.1254
O	0.9177	1.6545	-0.6586
C	-0.0049	3.1802	1.1323
F	-0.4790	2.7953	2.3184
F	1.2259	3.6519	1.3021
F	-0.7773	4.1750	0.6732

Table S46. Refined Cartesian coordinates in Ångström (Å) for the experimentally-determined structure of **2** obtained *via* GED.

	x	*y*	*z*
O	0.0000	0.0000	-1.9128
Sn	-0.0043	1.7509	-1.2314
Sn	0.0043	-1.7509	-1.2314
O	-1.5611	1.1394	0.2156
C	-1.9409	-0.0048	0.5709
O	-1.5555	-1.1471	0.2156
C	-3.0769	-0.0076	1.6258
F	-4.2489	0.4035	1.0991
F	-3.2855	-1.2265	2.1318
F	-2.7513	0.8360	2.6126
O	1.5611	-1.1394	0.2156
C	1.9409	0.0048	0.5709
O	1.5555	1.1471	0.2156
C	3.0769	0.0076	1.6258
F	4.2489	-0.4035	1.0991
F	3.2855	1.2265	2.1318
F	2.7513	-0.8360	2.6126

Density Functional Theory (DFT) and Gas-Phase Electron Diffraction (GED) of 6

Table S47. Summary of experimental parameters relating to GED data collection for **6**.

Dataset Type	Short	Long
Nozzle-to-Image-Plate Distance / mm	233.5	486.0
Electron Wavelength / pm	5.85	5.85
$T_{\text{nozzle, av}}$ / K	408	408
$T_{\text{sample, av}}$ / K	398	398
Exposure Time / s	240	120

Table S48. Optimised Cartesian coordinates in Ångström (Å) and energy, E_{M06}, in atomic units (a.u) of **6** as calculated at the M06/def2-SVP level.

E_{M06} = -2316.91349099							
Sn	0.000000	0.000000	0.000000	O	2.168435	0.000000	-0.317988
O	0.000000	2.168435	0.317988	C	2.394408	0.000000	0.926142
C	0.000000	2.394408	-0.926142	O	1.456604	0.000000	1.739939
O	0.000000	1.456604	-1.739939	C	3.859818	0.000000	1.381088
C	0.000000	3.859818	-1.381088	F	3.951314	0.000000	2.691732
F	0.000000	3.951314	-2.691732	F	4.45773	-1.076801	0.900932
F	1.076801	4.45773	-0.900932	F	4.45773	1.076801	0.900932
F	-1.076801	4.45773	-0.900932	O	-2.168435	0.000000	-0.317988
O	0.000000	-2.168435	0.317988	C	-2.394408	0.000000	0.926142
C	0.000000	-2.394408	-0.926142	O	-1.456604	0.000000	1.739939
O	0.000000	-1.456604	-1.739939	C	-3.859818	0.000000	1.381088
C	0.000000	-3.859818	-1.381088	F	-3.951314	0.000000	2.691732
F	0.000000	-3.951314	-2.691732	F	-4.45773	-1.076801	0.900932
F	1.076801	-4.45773	-0.900932	F	-4.45773	1.076801	0.900932
F	-1.076801	-4.45773	-0.900932				

Table S49. Optimised Cartesian coordinates in Ångström (Å) and energy, E_{M06}, in atomic units (a.u) of **6** as calculated at the M06/def2-TZVP level.

E_{M06} = -2316.91349099							
Sn	0.000000	0.000000	0.000000	O	2.135398	0.000000	-0.324253
O	0.000000	2.135398	0.324253	C	2.365574	0.000000	0.917616
C	0.000000	2.365574	-0.917616	O	1.436904	0.000000	1.736140
O	0.000000	1.436904	-1.736140	C	3.837518	0.000000	1.366232
C	0.000000	3.837518	-1.366232	F	3.935414	0.000000	2.675278
F	0.000000	3.935414	-2.675278	F	4.437258	-1.075501	0.885907
F	1.075501	4.437258	-0.885907	F	4.437258	1.075501	0.885907
F	-1.075501	4.437258	-0.885907	O	-2.135398	0.000000	-0.324253
O	0.000000	-2.135398	0.324253	C	-2.365574	0.000000	0.917616
C	0.000000	-2.365574	-0.917616	O	-1.436904	0.000000	1.736140
O	0.000000	-1.436904	-1.736140	C	-3.837518	0.000000	1.366232
C	0.000000	-3.837518	-1.366232	F	-3.935414	0.000000	2.675278
F	0.000000	-3.935414	-2.675278	F	-4.437258	-1.075501	0.885907
F	1.075501	-4.437258	-0.885907	F	-4.437258	1.075501	0.885907
F	-1.075501	-4.437258	-0.885907				

Table S50. Optimised Cartesian coordinates in Ångström (Å) and energy, E_{M06}, in atomic units (a.u) of **6** as calculated at the M06/def2-QZVP level.

E_{M06} = -2319.49251729			
Sn	0.000000	0.000000	0.000000
O	0.000000	2.133713	0.324164
C	0.000000	2.364684	-0.916574
O	0.000000	1.437195	-1.734956
C	0.000000	3.837399	-1.364268
F	0.000000	3.936537	-2.672712
F	1.075175	4.436618	-0.883462
F	-1.075175	4.436618	-0.883462
O	0.000000	-2.133713	0.324164
C	0.000000	-2.364684	-0.916574
O	0.000000	-1.437195	-1.734956
C	0.000000	-3.837399	-1.364268
F	0.000000	-3.936537	-2.672712
F	1.075175	-4.436618	-0.883462
F	-1.075175	-4.436618	-0.883462
O	2.133713	0.000000	-0.324164
C	2.364684	0.000000	0.916574
O	1.437195	0.000000	1.734956
C	3.837399	0.000000	1.364268
F	3.936537	0.000000	2.672712
F	4.436618	-1.075175	0.883462
F	4.436618	1.075175	0.883462
O	-2.133713	0.000000	-0.324164
C	-2.364684	0.000000	0.916574
O	-1.437195	0.000000	1.734956
C	-3.837399	0.000000	1.364268
F	-3.936537	0.000000	2.672712
F	-4.436618	-1.075175	0.883462
F	-4.436618	1.075175	0.883462

Table S51. Optimised Cartesian coordinates in Ångström (Å) and energy, E_{M11}, in atomic units (a.u) of **6** as calculated at the M11/def2-SVP level.

E_{M11} = -2316.77650596							
Sn	0.000000	0.000000	0.000000	O	2.132375	0.000000	-0.319500
O	0.000000	2.132375	0.319500	C	2.380689	0.000000	0.924499
C	0.000000	2.380689	-0.924499	O	1.446277	0.000000	1.738112
O	0.000000	1.446277	-1.738112	C	3.854386	0.000000	1.369494
C	0.000000	3.854386	-1.369494	F	3.944764	0.000000	2.688753
F	0.000000	3.944764	-2.688753	F	4.454812	-1.083464	0.884641
F	1.083464	4.454812	-0.884641	F	4.454812	1.083464	0.884641
F	-1.083464	4.454812	-0.884641	O	-2.132375	0.000000	-0.319500
O	0.000000	-2.132375	0.319500	C	-2.380689	0.000000	0.924499
C	0.000000	-2.380689	-0.924499	O	-1.446277	0.000000	1.738112
O	0.000000	-1.446277	-1.738112	C	-3.854386	0.000000	1.369494
C	0.000000	-3.854386	-1.369494	F	-3.944764	0.000000	2.688753
F	0.000000	-3.944764	-2.688753	F	-4.454812	-1.083464	0.884641
F	1.083464	-4.454812	-0.884641	F	-4.454812	1.083464	0.884641
F	-1.083464	-4.454812	-0.884641				

Table S52. Optimised Cartesian coordinates in Ångström (Å) and energy, E_{M11}, in atomic units (a.u) of **6** as calculated at the M11/def2-TZVP level.

E_{M11} = -2319.47858823			
Sn	0.000000	0.000000	0.000000
O	0.000000	2.108306	0.323714
C	0.000000	2.357560	-0.920132
O	0.000000	1.432383	-1.740580
C	0.000000	3.835325	-1.358709
F	0.000000	3.935929	-2.680973
F	1.086216	4.439761	-0.871154
F	-1.086216	4.439761	-0.871154
O	0.000000	-2.108306	0.323714
C	0.000000	-2.357560	-0.920132
O	0.000000	-1.432383	-1.740580
C	0.000000	-3.835325	-1.358709
F	0.000000	-3.935929	-2.680973
F	1.086216	-4.439761	-0.871154
F	-1.086216	-4.439761	-0.871154
O	2.108306	0.000000	-0.323714
C	2.357560	0.000000	0.920132
O	1.432383	0.000000	1.740580
C	3.835325	0.000000	1.358709
F	3.935929	0.000000	2.680973
F	4.439761	-1.086216	0.871154
F	4.439761	1.086216	0.871154
O	-2.108306	0.000000	-0.323714
C	-2.357560	0.000000	0.920132
O	-1.432383	0.000000	1.740580
C	-3.835325	0.000000	1.358709
F	-3.935929	0.000000	2.680973
F	-4.439761	-1.086216	0.871154
F	-4.439761	1.086216	0.871154

Table S53. Optimised Cartesian coordinates in Ångström (Å) and energy, E_{M11}, in atomic units (a.u) of **6** as calculated at the M11/def2-QZVP level.

E_{M11} = -2319.66659259							
Sn	0.000000	0.000000	0.000000	O	2.109252	0.000000	-0.326053
O	0.000000	2.109252	0.326053	C	2.357633	0.000000	0.916728
C	0.000000	2.357633	-0.916728	O	1.432524	0.000000	1.737270
O	0.000000	1.432524	-1.737270	C	3.835078	0.000000	1.357267
C	0.000000	3.835078	-1.357267	F	3.934629	0.000000	2.679227
F	0.000000	3.934629	-2.679227	F	4.440013	-1.086074	0.870573
F	1.086074	4.440013	-0.870573	F	4.440013	1.086074	0.870573
F	-1.086074	4.440013	-0.870573	O	-2.109252	0.000000	-0.326053
O	0.000000	-2.109252	0.326053	C	-2.357633	0.000000	0.916728
C	0.000000	-2.357633	-0.916728	O	-1.432524	0.000000	1.737270
O	0.000000	-1.432524	-1.737270	C	-3.835078	0.000000	1.357267
C	0.000000	-3.835078	-1.357267	F	-3.934629	0.000000	2.679227
F	0.000000	-3.934629	-2.679227	F	-4.440013	-1.086074	0.870573
F	1.086074	-4.440013	-0.870573	F	-4.440013	1.086074	0.870573
F	-1.086074	-4.440013	-0.870573				

Table S54. Optimised Cartesian coordinates in Ångström (Å) and energy, $E_{SOGGA11X}$, in atomic units (a.u.) of **6** as calculated at the SOGGA11X/def2-SVP level.

$E_{SOGGA11X}$ = -2316.82492269			
Sn	0.000000	0.000000	0.000000
O	0.000000	2.156941	0.313825
C	0.000000	2.391863	-0.928596
O	0.000000	1.453111	-1.738483
C	0.000000	3.858116	-1.393900
F	0.000000	3.935733	-2.708341
F	1.078452	4.465536	-0.922910
F	-1.078452	4.465536	-0.922910
O	0.000000	-2.156941	0.313825
C	0.000000	-2.391863	-0.928596
O	0.000000	-1.453111	-1.738483
C	0.000000	-3.858116	-1.393900
F	0.000000	-3.935733	-2.708341
F	1.078452	-4.465536	-0.922910
F	-1.078452	-4.465536	-0.922910
O	2.156941	0.000000	-0.313825
C	2.391863	0.000000	0.928596
O	1.453111	0.000000	1.738483
C	3.858116	0.000000	1.393900
F	3.935733	0.000000	2.708341
F	4.465536	-1.078452	0.922910
F	4.465536	1.078452	0.922910
O	-2.156941	0.000000	-0.313825
C	-2.391863	0.000000	0.928596
O	-1.453111	0.000000	1.738483
C	-3.858116	0.000000	1.393900
F	-3.935733	0.000000	2.708341
F	-4.465536	-1.078452	0.922910
F	-4.465536	1.078452	0.922910

Table S55. Optimised Cartesian coordinates in Ångström (Å) and energy, $E_{SOGGA11X}$, in atomic units (a.u) of **6** as calculated at the SOGGA11X/def2-TZVP level.

$E_{SOGGA11X}$ = -2319.40649637							
Sn	0.000000	0.000000	0.000000	O	2.121597	0.000000	-0.323822
O	0.000000	2.121597	0.323822	C	2.361864	0.000000	0.918005
C	0.000000	2.361864	-0.918005	O	1.429048	0.000000	1.733017
O	0.000000	1.429048	-1.733017	C	3.835584	0.000000	1.375491
C	0.000000	3.835584	-1.375491	F	3.924326	0.000000	2.690782
F	0.000000	3.924326	-2.690782	F	4.444543	-1.079189	0.901714
F	1.079189	4.444543	-0.901714	F	4.444543	1.079189	0.901714
F	-1.079189	4.444543	-0.901714	O	-2.121597	0.000000	-0.323822
O	0.000000	-2.121597	0.323822	C	-2.361864	0.000000	0.918005
C	0.000000	-2.361864	-0.918005	O	-1.429048	0.000000	1.733017
O	0.000000	-1.429048	-1.733017	C	-3.835584	0.000000	1.375491
C	0.000000	-3.835584	-1.375491	F	-3.924326	0.000000	2.690782
F	0.000000	-3.924326	-2.690782	F	-4.444543	-1.079189	0.901714
F	1.079189	-4.444543	-0.901714	F	-4.444543	1.079189	0.901714
F	-1.079189	-4.444543	-0.901714				

Table S56. Optimised Cartesian coordinates in Ångström (Å) and energy, $E_{SOGGA11X}$, in atomic units (a.u) of **6** as calculated at the SOGGA11X/def2-QZVP level.

$E_{SOGGA11X}$ = -2319.50412150			
Sn	0.000000	0.000000	0.000000
O	0.000000	2.120466	0.323860
C	0.000000	2.360683	-0.917081
O	0.000000	1.428527	-1.731776
C	0.000000	3.834530	-1.375045
F	0.000000	3.922812	-2.689624
F	1.078579	4.443525	-0.901708
F	-1.078579	4.443525	-0.901708
O	0.000000	-2.120466	0.323860
C	0.000000	-2.360683	-0.917081
O	0.000000	-1.428527	-1.731776
C	0.000000	-3.834530	-1.375045
F	0.000000	-3.922812	-2.689624
F	1.078579	-4.443525	-0.901708
F	-1.078579	-4.443525	-0.901708
O	2.120466	0.000000	-0.323860
C	2.360683	0.000000	0.917081
O	1.428527	0.000000	1.731776
C	3.834530	0.000000	1.375045
F	3.922812	0.000000	2.689624
F	4.443525	-1.078579	0.901708
F	4.443525	1.078579	0.901708
O	-2.120466	0.000000	-0.323860
C	-2.360683	0.000000	0.917081
O	-1.428527	0.000000	1.731776
C	-3.834530	0.000000	1.375045
F	-3.922812	0.000000	2.689624
F	-4.443525	-1.078579	0.901708
F	-4.443525	1.078579	0.901708

Table S57. Optimised Cartesian coordinates in Ångström (Å) and energy, $E_{SOGGA11X}$, in atomic units (a.u) of **6** as calculated at the SOGGA11X/DZP-DKH level.

$E_{SOGGA11-X}$ = -8276.16859272							
Sn	0.000000	0.000000	-0.000181	O	2.090650	0.000000	-0.321054
O	0.000000	2.090607	0.320971	C	2.379700	0.000000	0.922964
C	0.000000	2.379824	-0.923008	O	1.486575	0.000000	1.776924
O	0.000000	1.486813	-1.777088	C	3.874553	0.000000	1.298731
C	0.000000	3.874727	-1.298575	F	4.031611	0.000000	2.610264
F	0.000000	4.031960	-2.610086	F	4.458057	-1.081891	0.791020
F	1.081891	4.458163	-0.790785	F	4.458057	1.081891	0.791020
F	-1.081891	4.458163	-0.790785	O	-2.090650	0.000000	-0.321054
O	0.000000	-2.090607	0.320971	C	-2.379700	0.000000	0.922964
C	0.000000	-2.379824	-0.923008	O	-1.486575	0.000000	1.776924
O	0.000000	-1.486813	-1.777088	C	-3.874553	0.000000	1.298731
C	0.000000	-3.874727	-1.298575	F	-4.031611	0.000000	2.610264
F	0.000000	-4.031960	-2.610086	F	-4.458057	-1.081891	0.791020
F	1.081891	-4.458163	-0.790785	F	-4.458057	1.081891	0.791020
F	-1.081891	-4.458163	-0.790785				

Table S58. Optimised Cartesian coordinates in Ångström (Å) and energy, $E_{SOGGA11X}$, in atomic units (a.u) of **6** as calculated at the SOGGA11X/TZP-DKH level.

$E_{SOGGA11-X}$ = -8276.16859272							
Sn	0.000000	0.000000	-0.000143	O	-2.100459	0.000000	-0.391210
O	0.000000	-2.100417	0.391147	C	-2.365911	0.000000	0.844450
C	0.000000	-2.366001	-0.844484	O	-1.457366	0.000000	1.684767
O	0.000000	-1.457545	-1.684898	C	-3.849421	0.000000	1.267085
C	0.000000	-3.849556	-1.266962	F	-3.968170	0.000000	2.579393
F	0.000000	-3.968444	-2.579257	F	-4.445986	1.079058	0.779533
F	-1.079058	-4.446069	-0.779346	F	-4.445986	-1.079058	0.779533
F	1.079058	-4.446069	-0.779346	O	2.100459	0.000000	-0.391210
O	0.000000	2.100417	0.391147	C	2.365911	0.000000	0.844450
C	0.000000	2.366001	-0.844484	O	1.457366	0.000000	1.684767
O	0.000000	1.457545	-1.684898	C	3.849421	0.000000	1.267085
C	0.000000	3.849556	-1.266962	F	3.968170	0.000000	2.579393
F	0.000000	3.968444	-2.579257	F	4.445986	1.079058	0.779533
F	-1.079058	4.446069	-0.779346	F	4.445986	-1.079058	0.779533
F	1.079058	4.446069	-0.779346				

Table S59. Definitions of the parameters used in the parameterized molecular model of **6**.

	Parameter	Definition
p_1	rSn-O^a	$^1/_2$ rSn(1)-O(2) + $^1/_2$ rSn(1)-O(4)
p_2	rSn-O^b	rSn(1)-O(4) – rSn(1)-O(2)
p_3	rSn-C	rSn(1)-C(3)
p_4	rC-O^a	$^1/_2$ rO(2)-C(3) + $^1/_2$ rO(4)-C(3)
p_5	rC-O^b	rO(2)-C(3) – rO(4)-C(3)
p_6	rC-C	rC(3)-C(5)
p_7	rC-F^a	$^1/_3$ rC(5)-F(6) + $^2/_3$ rC(5)-F(7)
p_8	rC-F^b	rC(5)-F(7) – rC(5)-F(6)
p_9	aO-C-C	aO(2)-C(3)-C(5)
p_{10}	aC-C-F^a	$^1/_3$ aC(3)-C(5)-F(6) + $^2/_3$ aC(3)-C(5)-F(7)
p_{11}	aC-C-F^b	aC(3)-C(5)-F(7) – aC(3)-C(5)-F(6)
p_{12}	aO-Sn-O	aO(2)-Sn(1)-O(9)

[a] Multiplicity-weighted average. [b] Refinable difference.

Table S60. Summary of experimental parameters relating to GED data reduction and refinement for **6**.

Dataset Type	Short	Long
Δs / nm^{-1}	2.0	1.0
s_{min} / nm^{-1}	90.0	54.0
sw_1 / nm^{-1}	104.0	68.0
sw_2 / nm^{-1}	240.0	101.0
s_{max} / nm^{-1}	262.0	114.0
Correlation parameter	0.4936	0.4975
Scale factor (k)	0.0023(1)	0.0010(1)

Table S61. Refined (r_{h1}) and theoretical[a] (r_e) parameter values[b] and SARACEN restraints[c] applied in the least-squares refinement of **6**.

	r_{h1}	r_e	Restraint
p_1	218.6(3)	218.2	–
p_2	8.8(6)	9.1	9.1(5)
p_3	125.5(2)	125.1	–
p_4	2.7(4)	2.6	2.6(3)
p_5	247.4(6)	251.2	–
p_6	153.1(3)	154.3	154.3(3)
p_7	133.0(2)	132.3	–
p_8	0.8(8)	0.8	0.8(6)
p_9	117.8(4)	118.0	118.0(3)
p_{10}	111.0(2)	110.0	–
p_{11}	1.7(3)	1.7	1.7(3)
p_{12}	158.7(3)	158.9	158.9(4)

[a] Calculations at the SOGGA11X/TZP-DKH level. [b] Interatomic distances (r) are tabulated in picometers (pm) and angles (a) are tabulated in degrees. [c] SARACEN restraint uncertainties are derived from sequential DFT geometry optimizations using the M06, M11 and SOGGA11X functionals and the def2-SVP, def2-TZVP and def2-QZVP basis sets.

Table S62. Least-squares correlation matrix[a] (×100) for **6**.

	p_1	p_3	p_5	p_7	p_{10}	u_1	u_{35}	u_{42}	u_{53}	k_1
p_1	100		81			55				
p_3		100							54	
p_5			100							
p_7				100	78					
p_{10}					100					51
u_1						100				57
u_{35}							100	63		
u_{42}								100		
u_{53}									100	55
k_1										100

[a] Only values ≥ 50% are tabulated. k_1 is a scale factor.

Table S63. Internuclear distances (r_a / pm), refined (u_{GED}) and theoretical (u_{h1}) amplitudes of vibration and restraints and distance corrections (k_{h1}) for **6**.[a]

Amp.	Atomic Pair	r_a	u_{GED}	Restraint	k_{h1}	u_{h1}
u_{25}	C(3)-O(4)	124.3(3)	1.7 (Tied to u_{53})	–	0.1	4.1
u_7	O(2)-C(3)	126.9(3)	1.8 (Tied to u_{53})	–	0.1	4.2
u_{52}	C(5)-F(6)	132.5(2)	2.4 (Tied to u_{53})	–	0.1	5.7
u_{53}	C(5)-F(7)	133.3(2)	2.8(4)	6.6(7)	0.2	6.6
u_{26}	C(3)-C(5)	152.9(3)	5.9(6)	5.0(5)	0.1	5.0
u_1	Sn(1)-O(2)	214.1(4)	6.0(3)	8.6(9)	0.2	8.6
u_{61}	F(6)...F(7)	214.4(2)	5.7 (Tied to u_1)	–	0.2	8.2
u_{67}	F(7)...F(8)	216.2(2)	6.5 (Tied to u_1)	–	0.2	9.4
u_8	O(2)...O(4)	221.7(5)	3.3 (Tied to u_1)	–	0.1	4.8
u_3	Sn(1)-O(4)	222.9(4)	7.5 (Tied to u_1)	–	0.3	10.8

Table S63. Internuclear distances (r_a / pm), refined (u_{GED}) and theoretical (u_{h1}) amplitudes of vibration and restraints and distance corrections (k_{h1}) for **6**,[a] *cont.*.

u_{28}	C(3)...F(7)	235.4(4)	8.7 (Tied to u_1)	–	0.3	12.6
u_{27}	C(3)...F(6)	237.1(4)	5.9 (Tied to u_1)	–	0.1	8.4
u_{40}	O(4)...C(5)	238.4(6)	4.6 (Tied to u_1)	–	0.1	6.6
u_9	O(2)...C(5)	240.1(6)	4.7 (Tied to u_1)	–	0.1	6.8
u_2	Sn(1)...C(3)	247.3(6)	4.1(2)	5.9(6)	0.1	5.9
u_{41}	O(4)...F(6)	262.0(9)	17.4 (Tied to u_2)	–	1.2	24.8
u_{20}	O(2)...O(18)	272.1(6)	12.6 (Tied to u_2)	–	0.5	18.0
u_{11}	O(2)...F(7)	284.8(7)	24.4 (Tied to u_2)	–	2.2	34.8
u_{19}	O(2)...C(17)	316.1(7)	19.9 (Tied to u_{42})	–	0.7	20.9
u_{18}	O(2)...O(16)	319.8(6)	21.6 (Tied to u_{42})	–	0.8	22.8
u_{42}	O(4)...F(7)	326.6(5)	37.6(17)	–	2.4	39.7
u_{43}	O(4)...O(11)	336.7(11)	19.3 (Tied to u_{35})	–	-0.1	16.6
u_{10}	O(2)...F(6)	351.6(5)	13.8 (Tied to u_{35})	–	0.2	11.9
u_{35}	C(3)...O(18)	351.7(7)	20.1(13)	17.4(17)	0.4	17.4
u_{34}	C(3)...C(17)	354.9(9)	21.8 (Tied to u_{35})	–	0.5	18.8
u_{47}	O(4)...O(18)	375.7(6)	20.7 (Tied to u_{35})	–	0.4	17.9
u_4	Sn(1)...C(5)	400.1(6)	10.2(5)	7.0(7)	0.1	7.0
u_{12}	O(2)...O(9)	401.4(10)	17.0 (Tied to u_4)	–	0.1	11.6
u_{30}	C(3)...O(11)	423.3(10)	19.5 (Tied to u_6)	–	0.3	15.1
u_{14}	O(2)...O(11)	429.5(7)	19.6 (Tied to u_6)	–	0.3	15.1
u_{21}	O(2)...C(19)	440.3(7)	39.1 (Tied to u_6)	–	1.0	30.1
u_{71}	F(7)...F(22)	450.7(12)	149.2 (Tied to u_6)	–	13.0	114.9
u_{24}	O(2)...F(22)	451.3(7)	88.1 (Tied to u_6)	–	5.0	67.9
u_{13}	O(2)...C(10)	459.6(10)	14.2 (Tied to u_6)	–	0.1	11.0
u_6	Sn(1)...F(7)	461.7(7)	24.3(7)	18.7(19)	0.4	18.7
u_{39}	C(3)...F(22)	465.0(9)	72.9 (Tied to u_6)	–	3.1	56.1
u_5	Sn(1)...F(6)	468.7(8)	17.9 (Tied to u_6)	–	0.2	13.8
u_{36}	C(3)...C(19)	475.1(8)	37.1 (Tied to u_6)	–	0.8	28.6
u_{51}	O(4)...F(22)	477.0(10)	49.4 (Tied to u_6)	–	1.4	38.1
u_{48}	O(4)...C(19)	478.2(7)	28.6 (Tied to u_6)	–	0.5	22.0
u_{22}	O(2)...F(20)	481.6(10)	58.9 (Tied to u_6)	–	2.0	45.4
u_{29}	C(3)...C(10)	485.4(12)	14.5 (Tied to u_6)	–	-0.3	11.2
u_{60}	C(5)...F(22)	530.5(10)	86.8 (Tied to u_{66})	–	5.2	77.6
u_{37}	C(3)...F(20)	544.5(9)	47.6 (Tied to u_{66})	–	1.5	42.6
u_{23}	O(2)...F(21)	547.3(7)	39.8 (Tied to u_{66})	–	1.2	35.6
u_{50}	O(4)...F(21)	548.6(9)	50.7 (Tied to u_{66})	–	1.8	45.3
u_{44}	O(4)...C(12)	568.4(11)	18.9 (Tied to u_{66})	–	0.3	16.9
u_{38}	C(3)...F(21)	570.4(8)	54.3 (Tied to u_{66})	–	2.0	48.5
u_{49}	O(4)...F(20)	570.7(6)	32.9 (Tied to u_{66})	–	0.7	29.4
u_{57}	C(5)...C(19)	571.6(8)	49.9 (Tied to u_{66})	–	1.6	44.6
u_{66}	F(6)...F(22)	578.9(11)	98.3(73)	87.8(88)	6.0	87.8

Table S63. Internuclear distances (r_a / pm), refined (u_{GED}) and theoretical (u_{h1}) amplitudes of vibration and restraints and distance corrections (k_{h1}) for **6**, [a] *cont.*.

u_{45}	O(4)...F(13)	595.7(15)	36.0 (Tied to u_{66})	–	0.9	32.2
u_{15}	O(2)...C(12)	612.0(9)	13.4 (Tied to u_{66})	–	0.1	12.0
u_{58}	C(5)...F(20)	633.5(8)	68.9 (Tied to u_{70})	–	2.8	61.7
u_{31}	C(3)...C(12)	637.8(12)	14.8 (Tied to u_{70})	–	0.1	13.2
u_{46}	O(4)...F(14)	639.1(10)	53.3 (Tied to u_{70})	–	1.9	47.7
u_{70}	F(7)...F(21)	640.8(10)	121.3(104)	108.5(109)	8.7	108.5
u_{17}	O(2)...F(14)	664.4(11)	30.6 (Tied to u_{70})	–	0.5	27.3
u_{59}	C(5)...F(21)	673.5(8)	80.4 (Tied to u_{70})	–	3.7	72.0
u_{16}	O(2)...F(13)	682.3(10)	23.3 (Tied to u_{70})	–	0.3	20.9
u_{32}	C(3)...F(13)	684.9(14)	30.5 (Tied to u_{70})	–	0.5	27.3
u_{33}	C(3)...F(14)	700.2(11)	43.9 (Tied to u_{70})	–	1.1	39.3
u_{64}	F(6)...F(20)	713.8(9)	80.9 (Tied to u_{70})	–	3.4	72.4
u_{65}	F(6)...F(21)	720.0(9)	103.0 (Tied to u_{70})	–	5.6	92.2
u_{72}	F(7)...F(28)	782.0(10)	93.9 (Tied to u_{63})	–	3.9	80.1
u_{54}	C(5)...C(12)	788.3(12)	18.8 (Tied to u_{63})	–	-0.3	16.0
u_{55}	C(5)...F(13)	829.3(17)	38.0 (Tied to u_{63})	–	0.6	32.4
u_{62}	F(6)...F(13)	848.6(25)	56.8 (Tied to u_{63})	–	0.7	48.4
u_{56}	C(5)...F(14)	850.5(11)	55.0 (Tied to u_{63})	–	1.3	46.8
u_{68}	F(7)...F(14)	893.8(14)	87.3 (Tied to u_{63})	–	3.1	74.4
u_{63}	F(6)...F(14)	897.3(14)	73.7(2)	–	2.3	62.8
u_{69}	F(7)...F(15)	922.6(13)	57.2 (Tied to u_{63})	–	1.3	48.8

[a] All values are tabulated in picometers (pm).

Table S64. Refined Cartesian coordinates in Ångström (Å) for the experimentally-determined structure of **6** obtained *via* GED.

	x	*y*	*z*
Sn	0.0000	0.0000	0.0000
O	2.0088	0.7434	0.0000
C	2.4318	-0.4525	0.0000
O	1.6930	-1.4509	0.0000
C	3.9468	-0.6736	0.0000
F	4.2630	-1.9596	0.0000
F	4.4972	-0.1230	1.0814
F	4.4972	-0.1230	-1.0814
O	-2.0088	0.7434	0.0000
C	-2.4318	-0.4525	0.0000
O	-1.6930	-1.4509	0.0000
C	-3.9468	-0.6736	0.0000
F	-4.2630	-1.9596	0.0000
F	-4.4972	-0.1230	1.0814
F	-4.4972	-0.1230	-1.0814
O	0.0000	-0.7434	2.0088
C	0.0000	0.4525	2.4318
O	0.0000	1.4509	1.6930
C	0.0000	0.6736	3.9468
F	0.0000	1.9596	4.2630
F	-1.0814	0.1230	4.4972
F	1.0814	0.1230	4.4972
O	0.0000	-0.7434	-2.0088
C	0.0000	0.4525	-2.4318
O	0.0000	1.4509	-1.6930
C	0.0000	0.6736	-3.9468
F	0.0000	1.9596	-4.2630
F	-1.0814	0.1230	-4.4972
F	1.0814	0.1230	-4.4972