

SUPPLEMENTARY INFORMATION

Diorganotin(IV) complexes of organoselenolato ligands with pyrazole moieties. Synthesis, structure and properties

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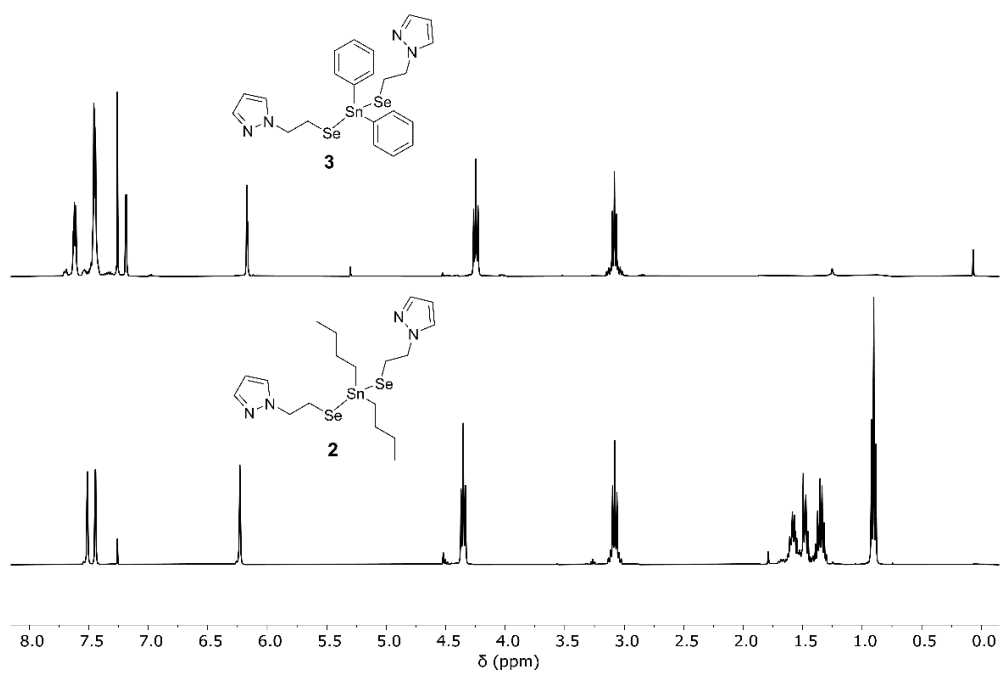


Figure S1. ^1H NMR spectra of compounds **2** and **3**, in CDCl_3

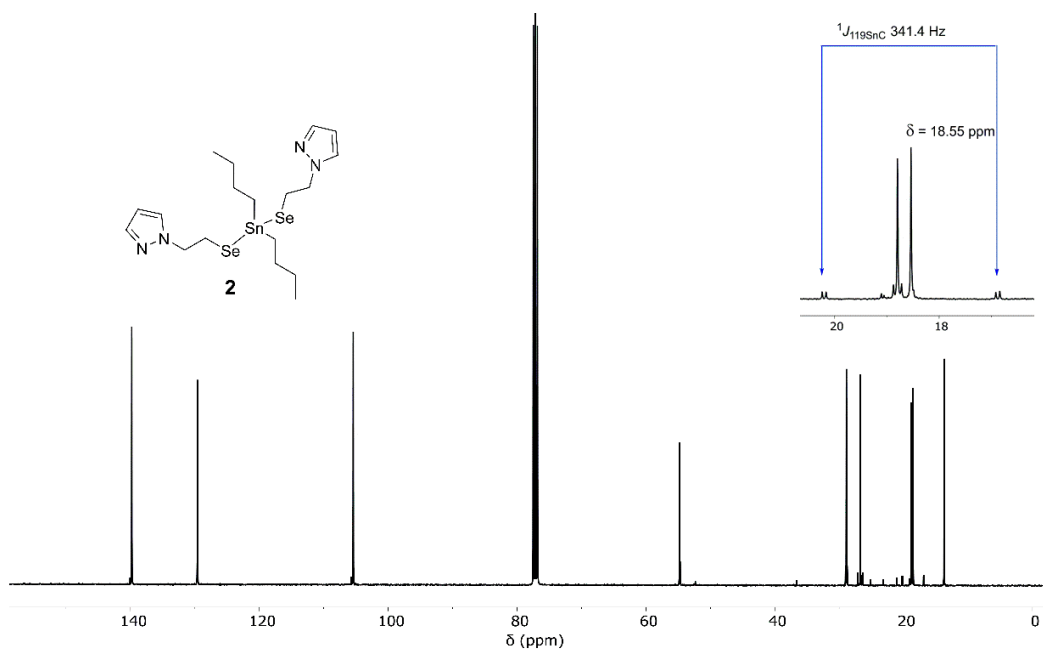


Figure S2. ^{13}C NMR spectrum of compound **2**, in CDCl_3

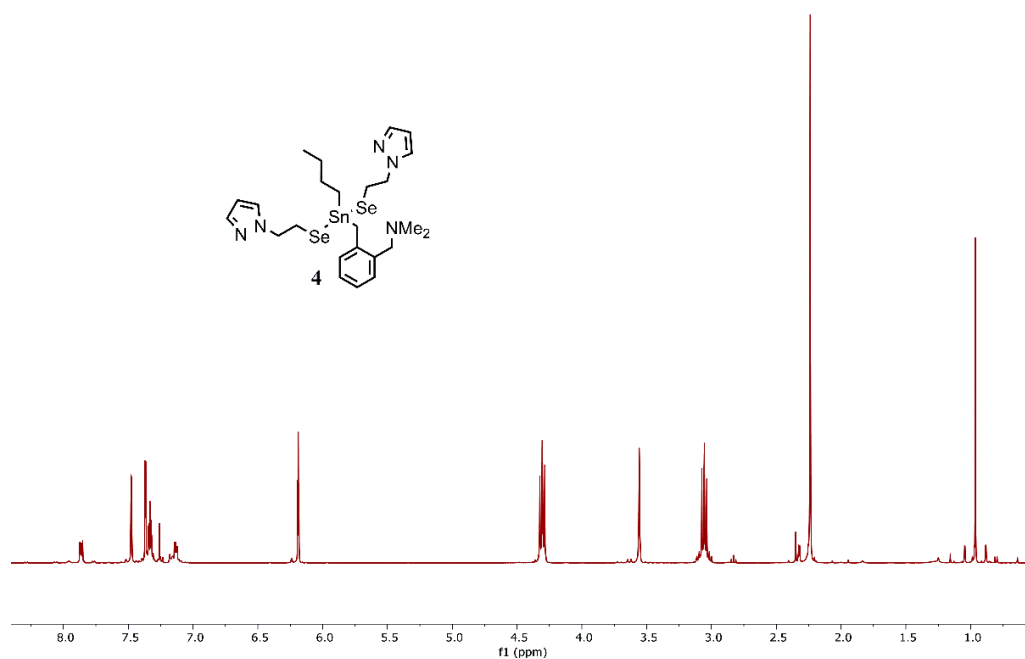


Figure S3. ^1H NMR spectrum of compound **4**, in CDCl_3

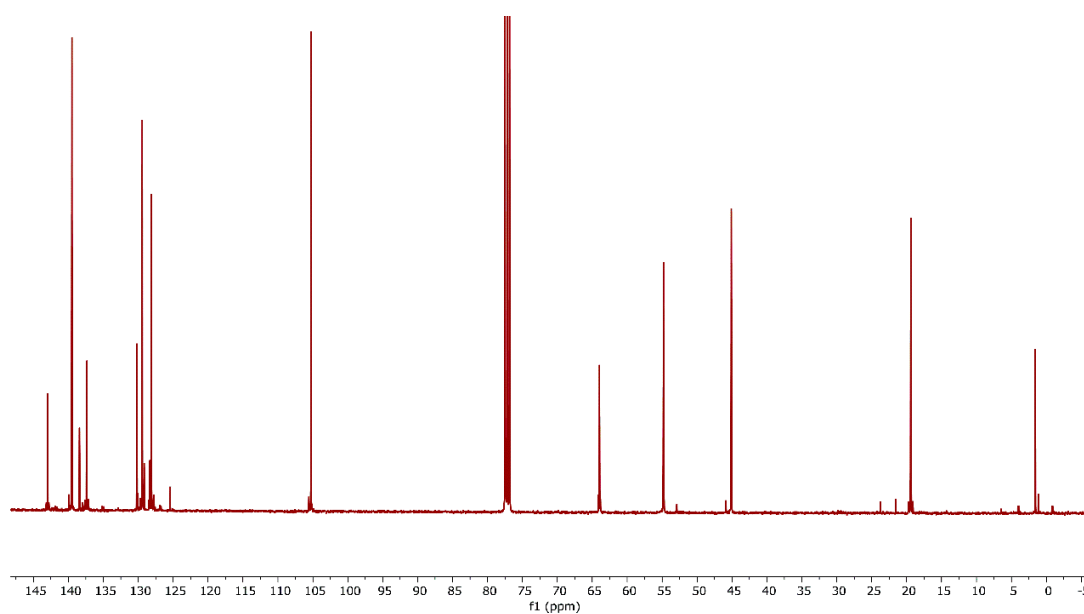


Figure S4. ^{13}C NMR spectrum of compound **4**, in CDCl_3

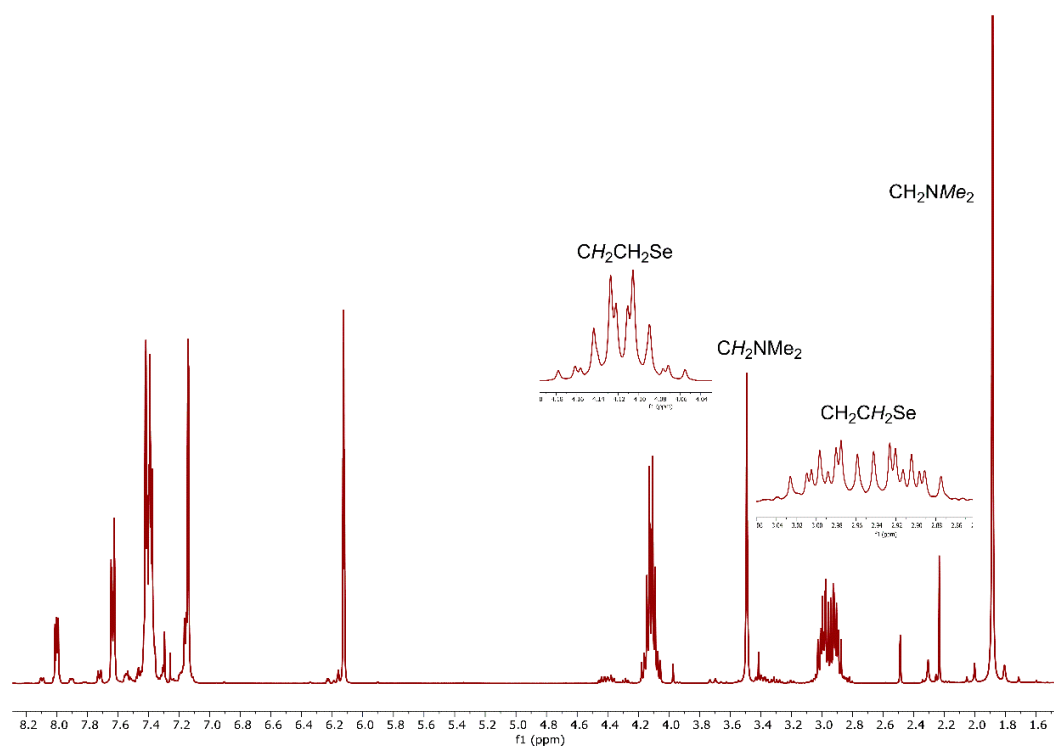


Figure S5. ^1H NMR spectrum of compound **6**, in CDCl_3

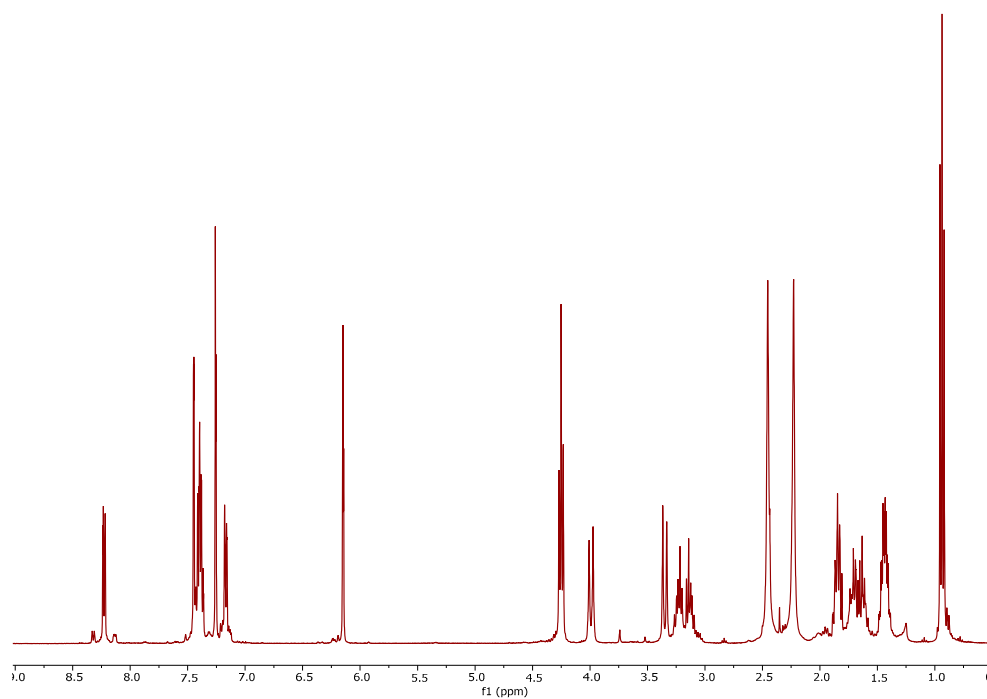


Figure S6. ^1H NMR spectrum of compound **7**, in CDCl_3

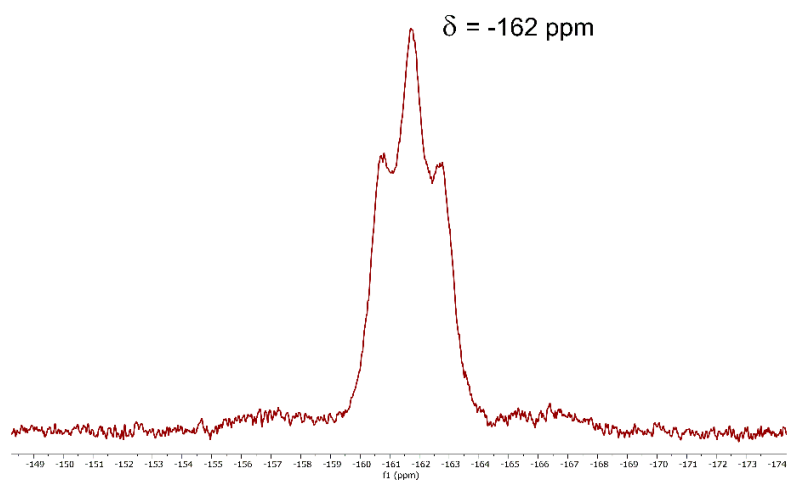


Figure S7. ^{119}Sn NMR resonance of $[2-(\text{Me}_2\text{NCH}_2)\text{C}_6\text{H}_4](\text{Me})\text{Sn}(\text{NCS})(\text{CH}_2\text{CH}_2\text{Se})$ (**9**), in CDCl_3

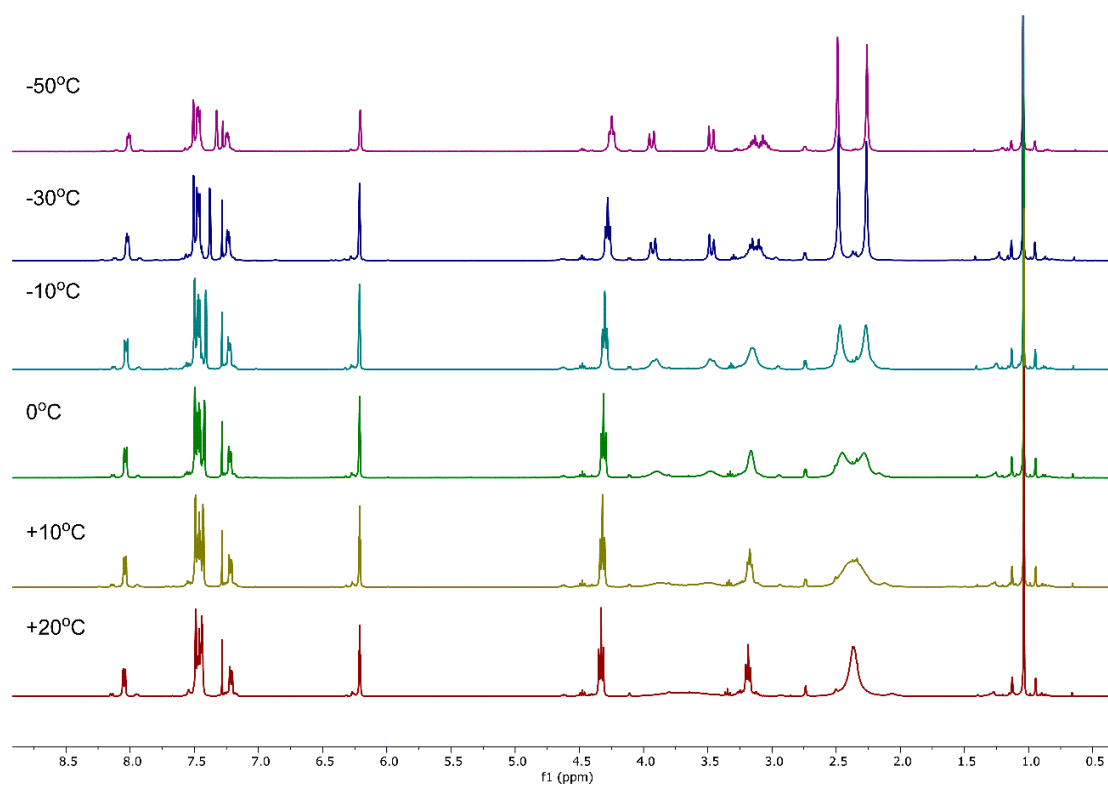


Figure S8. VT ^1H NMR spectra of compound **9**, in CDCl_3

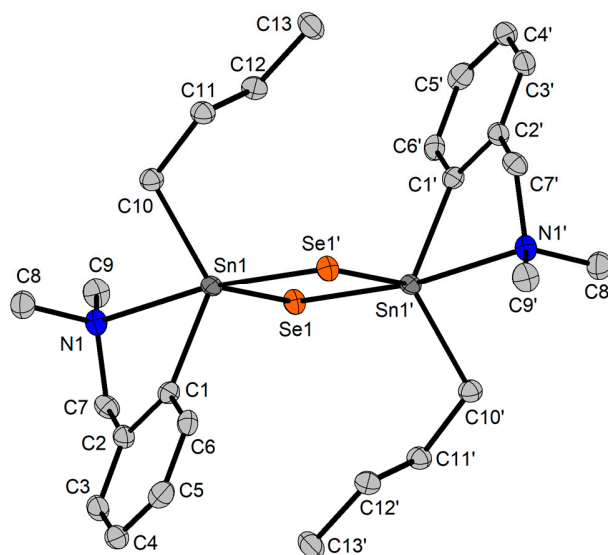


Figure S9. Thermal ellipsoids representation of a dimeric unit in compound **5-a**. Hydrogen atoms were omitted for clarity. Symmetry equivalent positions (1-x, 1-y, 1-z) are given by “prime”.

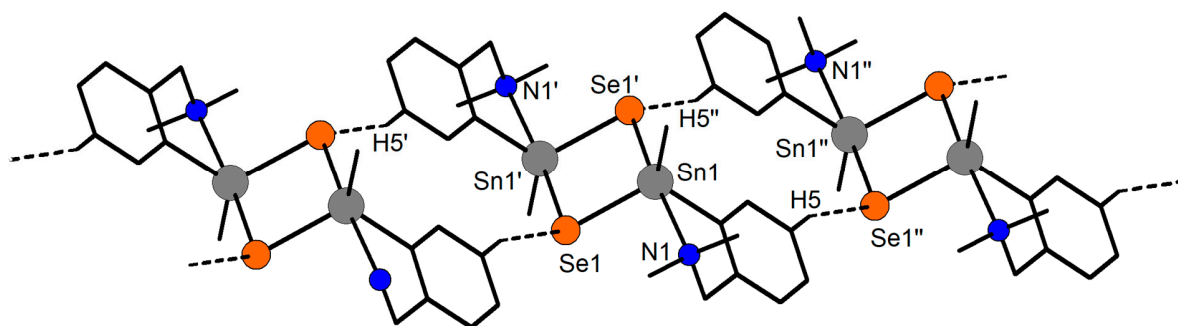


Figure S10. View along axis *c* of a chain in the crystal of **4-a**. Hydrogen atoms, except those involved in inter-dimers interactions were omitted for clarity. Symmetry equivalent positions (-x, 1-y, -z) and (1-x, 1-y, -z) are given by “prime” and “double prime”, respectively.

H5''...Se1' 3.028 Å, vs. $\Sigma r_{vdW}(H, Se)$ 3.10 Å

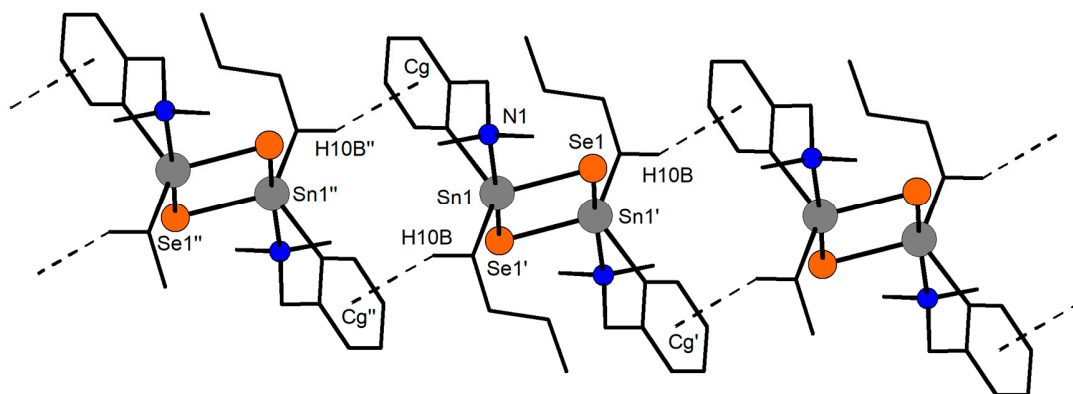


Figure S11. Best view of a chain in the crystal of **5-a**. Hydrogen atoms, except those involved in inter-dimers interactions were omitted for clarity. Symmetry equivalent positions (1-x, 1-y, 1-z) and (1-x, -y, 1-z) are given by “prime” and “double prime”, respectively.

H10B''...Cg 2.81 Å

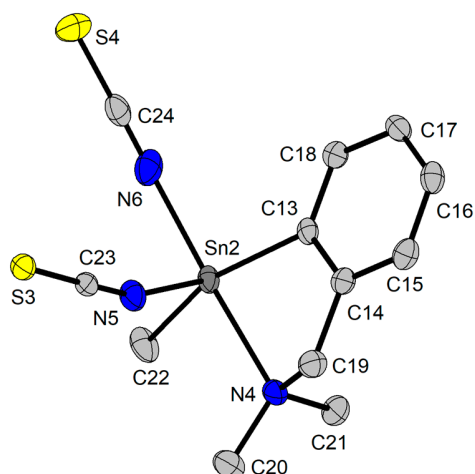


Figure S12. Thermal ellipsoids representation of molecule b in compound **8**. Hydrogen atoms were omitted for clarity.

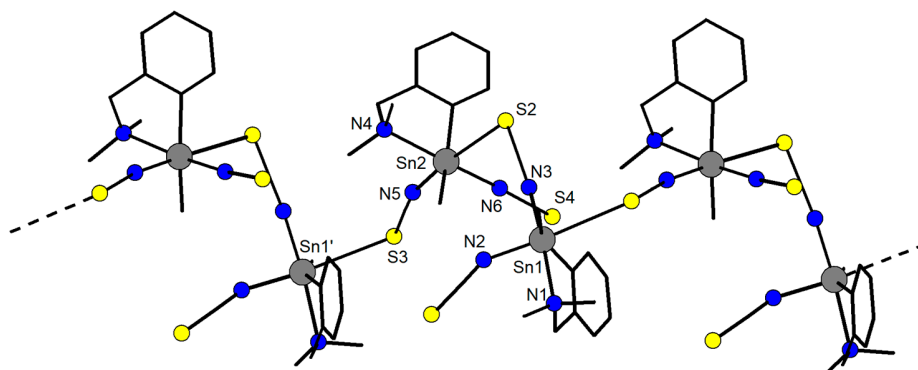


Figure S13. Best view of a chain in the crystal of **8**. Hydrogen atoms, except those involved in inter-dimers interactions were omitted for clarity. Symmetry equivalent positions (-x, 1-y, -z) are given by “prime”.

$S3 \cdots Sn1'$ 3.2876(6) Å, vs. $\Sigma r_{cov}(Sn,S)$ 2.44 Å and $\Sigma r_{vdw}(Sn,S)$ 4.31 Å

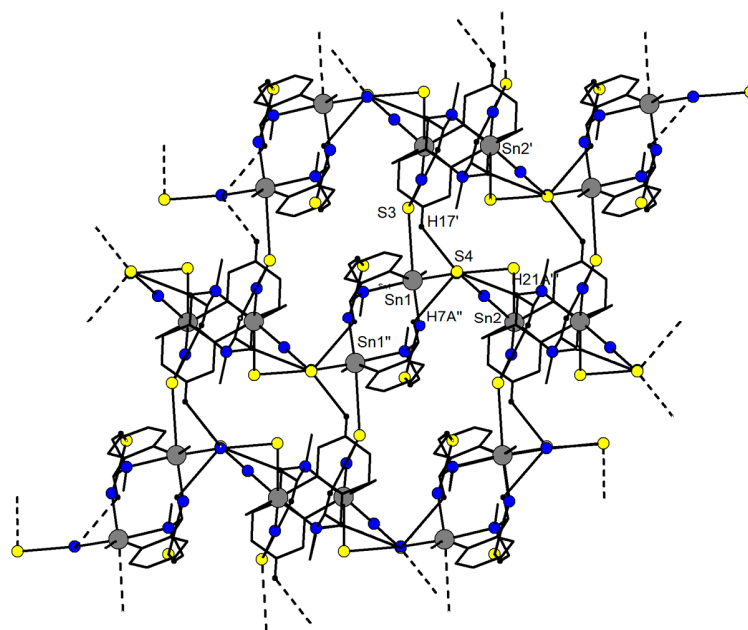


Figure S14. 3D network in the crystal of **8** (view along axis b)

Symmetry equivalent positions (1-x, 2-y, 1-z), (1/2-x, 1/2+y, 3/2-z), (3/2-x, 3/2+y, 3/2-z) are given by “prime”, “double prime”, and “triple prime”, respectively

$S4 \cdots H21A''$ 2.919 Å, vs. $\Sigma r_{vdw}(S,H)$ 3.10 Å
 $S4 \cdots H17'$ 2.717 Å $S4 \cdots H7A''$ 3.008 Å

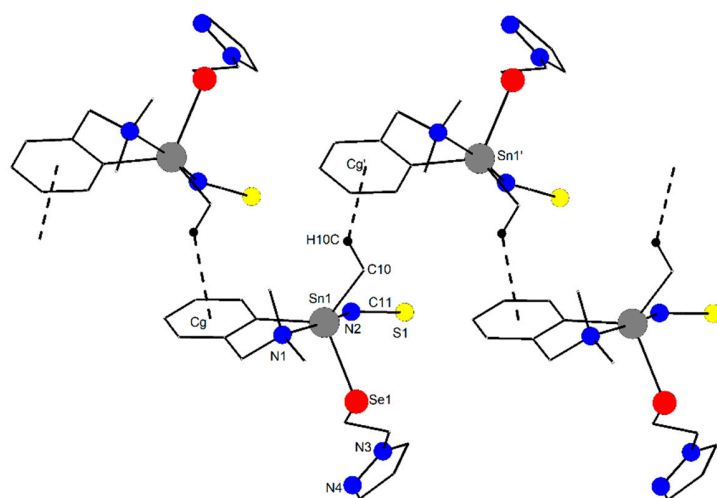


Figure S15. Best view of a chain in the crystal of **9**. Hydrogen atoms, except those involved in inter-dimers interactions were omitted for clarity. Symmetry equivalent positions ($1/2+x$, y , $1/2-z$) are given by “prime”.

$$\text{H10C} \cdots \text{Cg}' = 3.01 \text{ \AA}$$

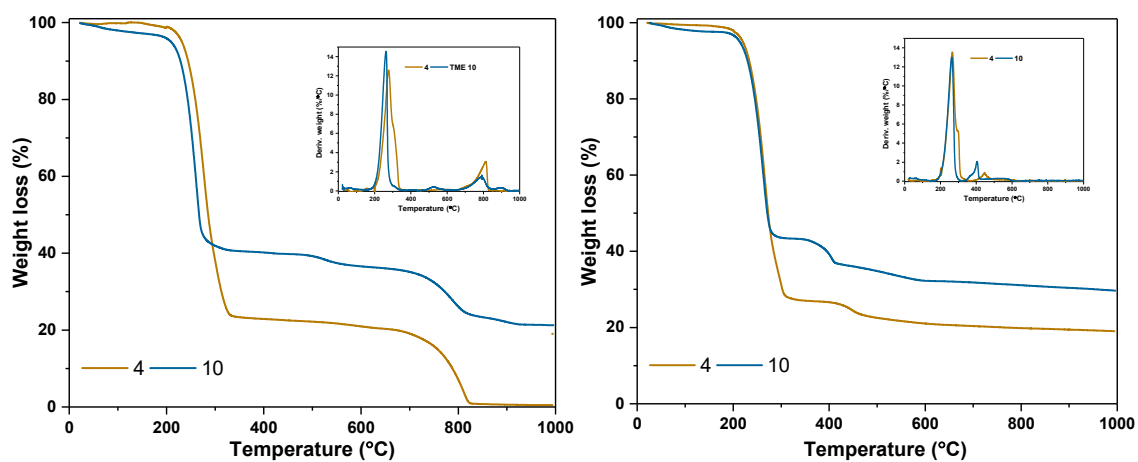


Figure S16. Thermogravimetric analysis data for compounds **4** and **10**, in argon (left), and in synthetic air (right)

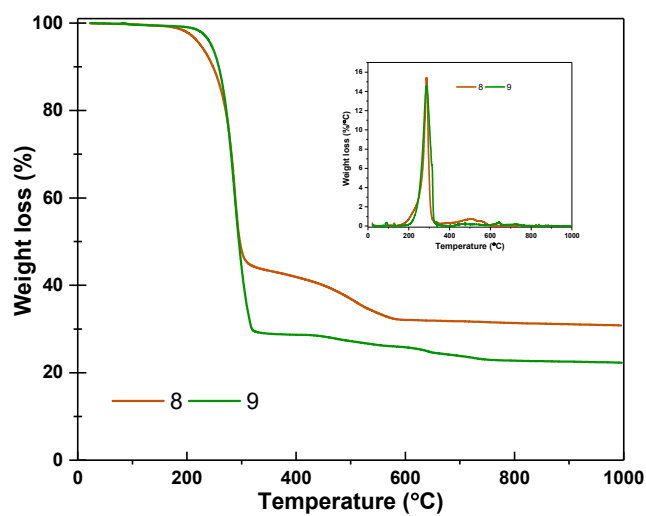


Figure S17. Thermogravimetric analysis data for compounds **8** and **9**, in synthetic air

Table S1. Crystallographic data for compounds **4-a** and **5-a**

	4-a	5-a
Empirical formula	C ₂₀ H ₃₀ N ₂ Se ₂ Sn ₂	C ₂₆ H ₄₂ N ₂ Se ₂ Sn ₂
Formula weight	693.76	777.91
Temperature	100.(2)	100.(2)
Wavelength	0.71073	0.71073
Crystal system	Monoclinic	Triclinic
Space group	P21/c	P-1
<i>a</i> [Å]	9.6290(11)	9.0921(6)
<i>b</i> [Å]	13.4804(14)	9.3314(6)
<i>c</i> [Å]	10.3069(12)	9.6736(6)
α [°]	90	115.972(2)
β [°]	117.85	93.422(2)
γ [°]	90	99.902(2)
Volume	1182.9(2)	718.36(8)
Z	2	1
Density (calculated)	1.948	1.798
Absorption coefficient	5.195	4.288
F(000)	664	380
Crystal size	0.129x0.214x0.228	0.181x 0.219x 0.223
Theta range for data collection	2.39 to 26.60	2.30 to 28.34
Index ranges	-12<= <i>h</i> <=12 -16<= <i>k</i> <=16 -12<= <i>l</i> <=12	-12<= <i>h</i> <=12 -12<= <i>k</i> <=12 -12<= <i>l</i> <=12
Reflections collected/unique	27714/2448	38409/3582
Completeness to theta max.	99 %	100 %
Absorption correction		
Refinement method		
Data / restraints / parameters	2448 / 0 / 121	3582 / 0 / 148
Goodness-of-fit on F ² -S	1.297	1.044
Final R indices [<i>I</i> >2sigma(<i>I</i>)]	R1 = 0.0129 wR2 = 0.0276	R1 = 0.0260 wR2 = 0.0492
R indices (all data)	R1 = 0.0136 wR2 = 0.0361	R1 = 0.0368 wR2 = 0.0525
Largest diff. peak and hole	0.432 and -0.417 e/Å ³	1.065 and -0.854 e/Å ³

Table S2. Crystallographic data for compounds **8** and **9**

	8	9
Empirical formula	C ₁₂ H ₁₅ N ₃ S ₂ Sn	C ₁₆ H ₂₂ N ₄ SSeSn
Formula weight	384.08	500.08
Temperature	100.(2)	100.(2)
Wavelength	0.71073	0.71073
Crystal system	Monoclinic	Orthorhombic
Space group	P21/n	Pbca
<i>a</i> [Å]	14.7835(8)	9.1223(10)
<i>b</i> [Å]	12.7152(6)	15.8529(16)
<i>c</i> [Å]	17.2721(9)	26.319(2)
α [°]	90	90
β [°]	112.643(2)	90
γ [°]	90	90
Volume	2996.5(3)	3806.1(7)
Z	8	8
Density (calculated)	1.703	1.745
Absorption coefficient	1.970	3.369
F(000)	1520	1968
Crystal size	0.117x0.136x 0.214	0.080x0.100x0.120
Theta range for data collection	2.05 to 26.41	2.68 to 28.28
Index ranges	-18<= <i>h</i> <=18 -15<= <i>k</i> <=15 -21<= <i>l</i> <=21	-12<= <i>h</i> <=12 -21<= <i>k</i> <=21 -35<= <i>l</i> <=34
Reflections collected/unique	65915 / 6138	75630 / 4696
Completeness to theta max.	99.8 %	99.6 %
Absorption correction	multi-scan	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	6138 / 0 / 331	4696 / 0 / 211
Goodness-of-fit on F ² -S	1.049	1.095
Final R indices [<i>I</i> >2sigma(<i>I</i>)]	R1 = 0.0179 wR2 = 0.0394	R1 = 0.0173 wR2 = 0.0349
R indices (all data)	R1 = 0.0194 wR2 = 0.0400	R1 = 0.0224 wR2 = 0.0374
Largest diff. peak and hole	1.066 and -0.662 e/Å ³	0.395 and -0.373 e/Å ³