Electronic Supplementary Information

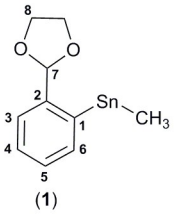
Novel mono- and bimetallic organotin(IV) compounds as potential linkers for coordination polymers†

Adrian-Alexandru Someşan,[a] Ioana Barbul, Sabina Mădălina Vieriu,[a] Richard A. Varga*[a] and Cristian Silvestru[a]

[a] *Departamentul de Chimie, Centrul de Chimie Supramoleculară Organică şi Organometalică (CCSOOM), Facultatea de Chimie şi Inginerie Chimică, Universitatea Babeş-Bolyai, RO-400028, Cluj-Napoca, Romania. E-mail:* richy@chem.ubbcluj.ro*; Fax: (+40) 264-590818; Tel: (+40) 264-593833*

Content

Numbering schemes for NMR resonance assignments



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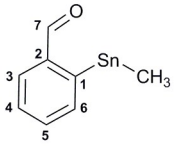

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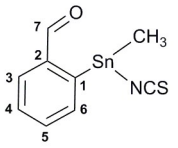

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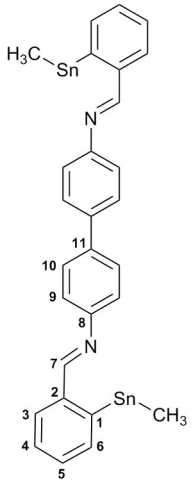

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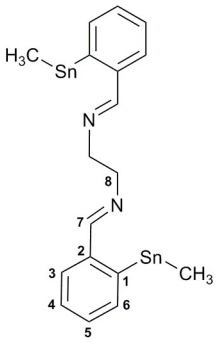

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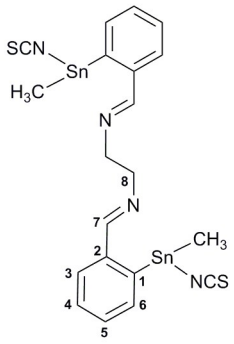

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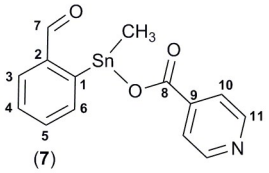

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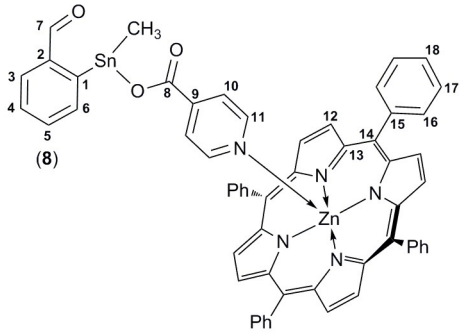

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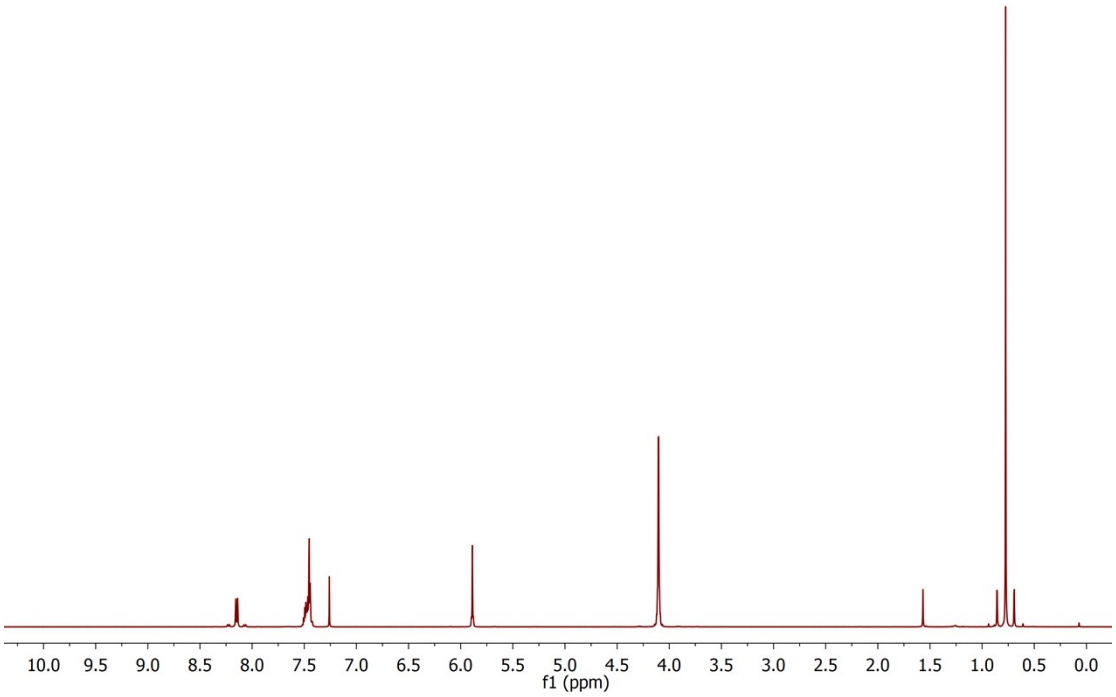

Figure S1. ^{1}H NMR ($CDCl_3$, 20 °C) spectrum of [2-{$(CH_2O)_2CH$}C_6H_4]Me_2SnCl (**1**).

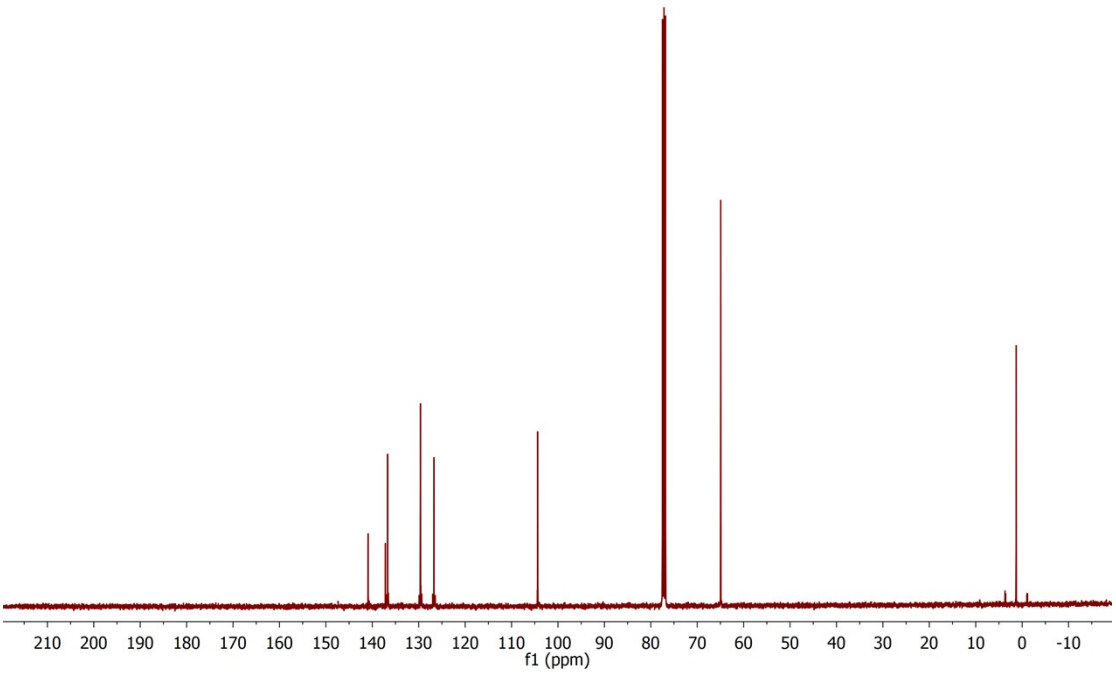

Figure S2. ^{13}C NMR ($CDCl_3$, 20 °C) spectrum of [2-{$(CH_2O)_2CH$}C_6H_4]Me_2SnCl (**1**).

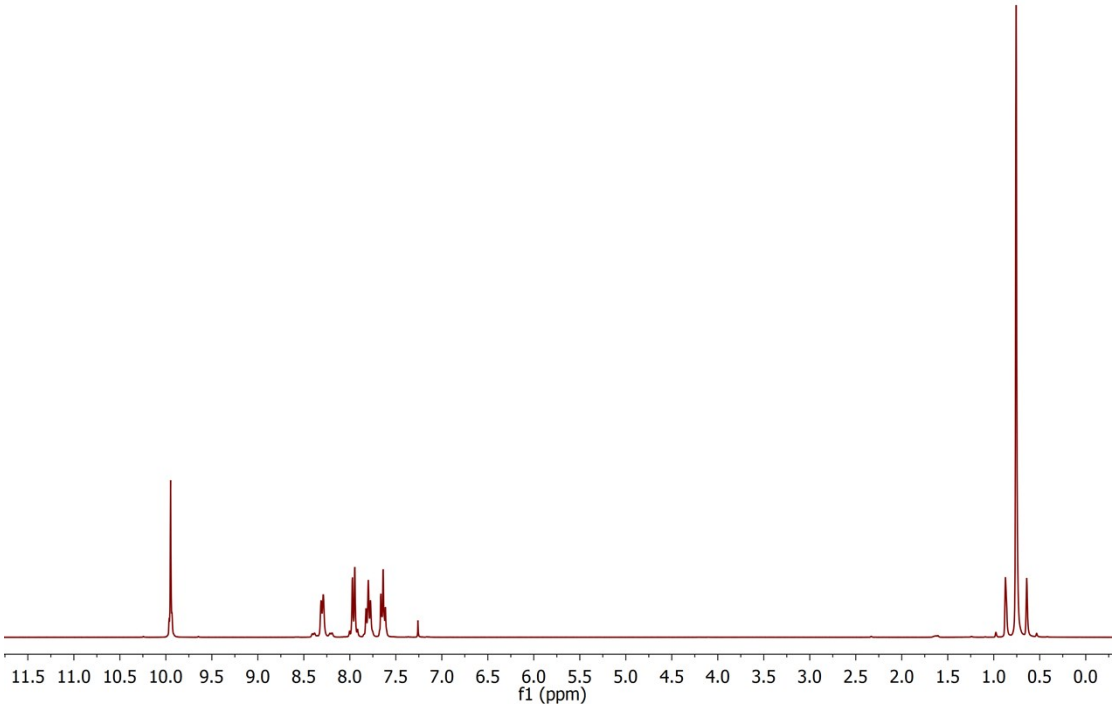

Figure S3. ^{1}H NMR ($CDCl_3$, 20 °C) spectrum of [2-(O=CH)C_6H_4]Me_2SnCl (**2**).

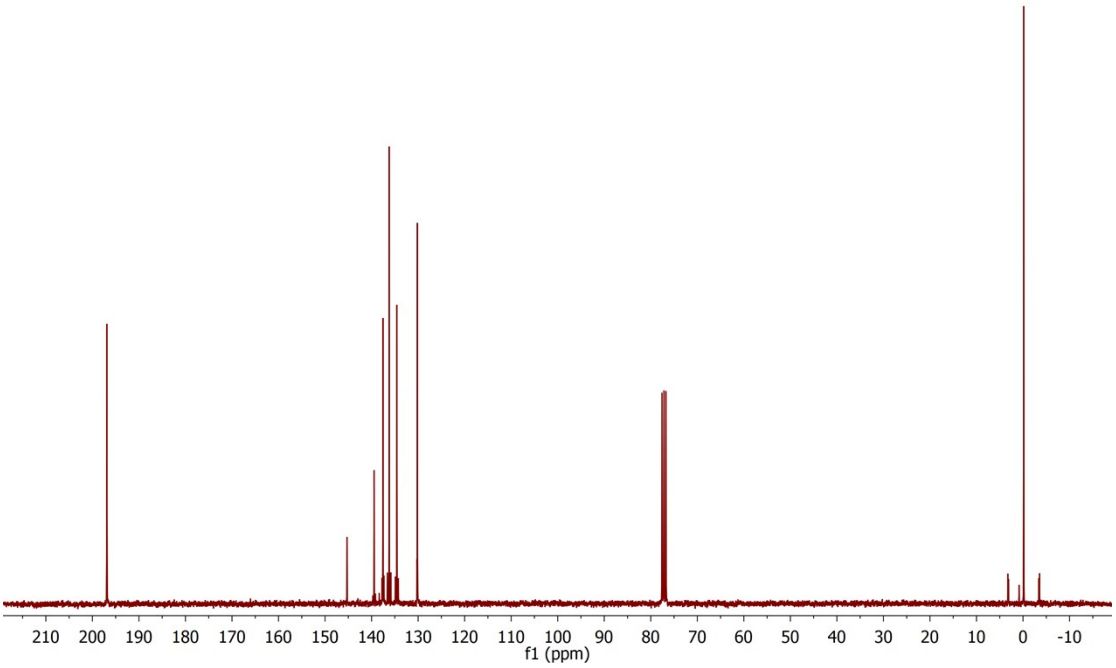

Figure S4. ^{13}C NMR ($CDCl_3$, 20 °C) spectrum of [2-(O=CH)C_6H_4]Me_2SnCl (**2**).

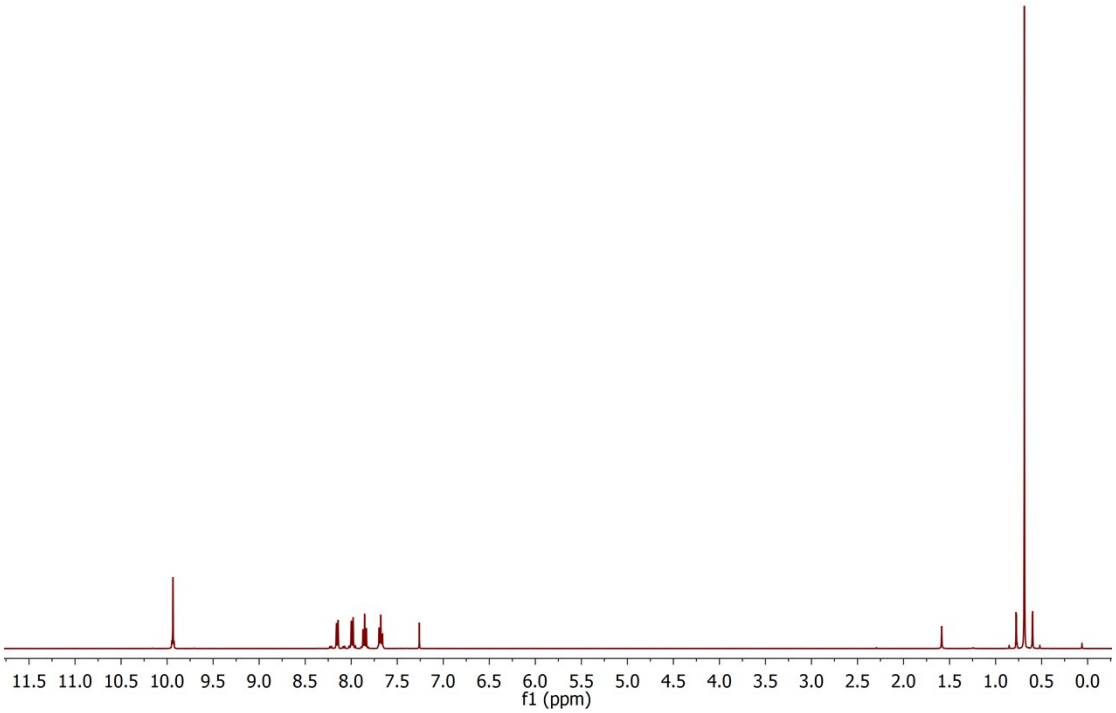

Figure S5. ^{1}H NMR ($CDCl_3$, 20 °C) spectrum of [2-(O=CH)C_6H_4]Me_2SnNCS (**3**).

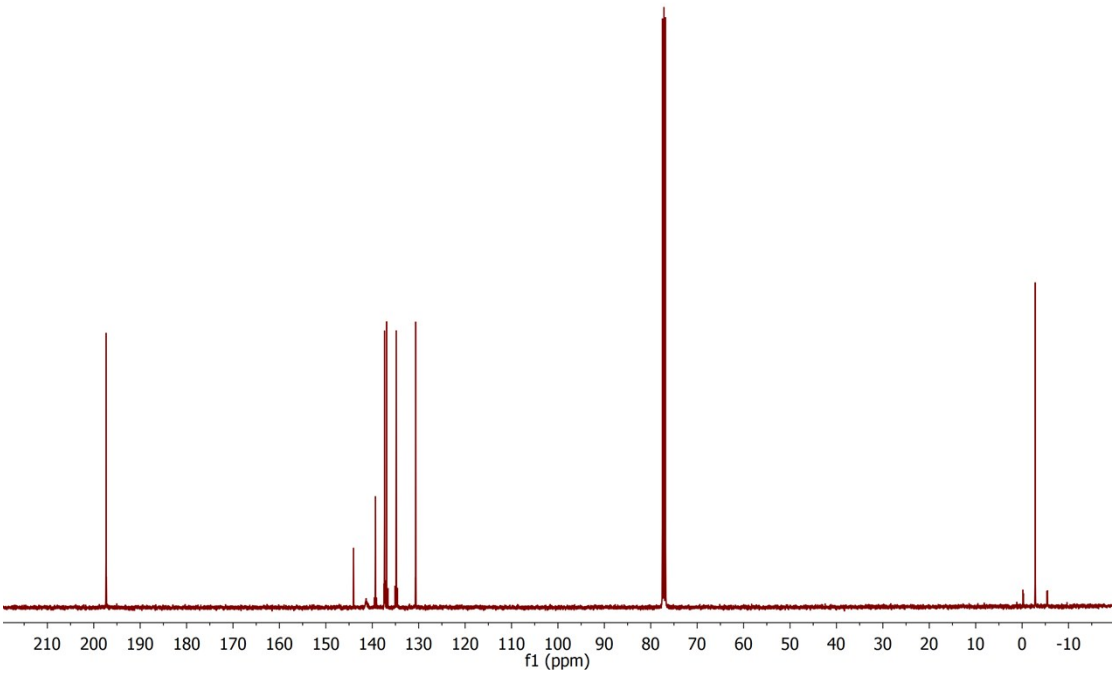

Figure S6. ^{13}C NMR ($CDCl_3$, 20 °C) spectrum of [2-(O=CH)C_6H_4]Me_2SnNCS (**3**).

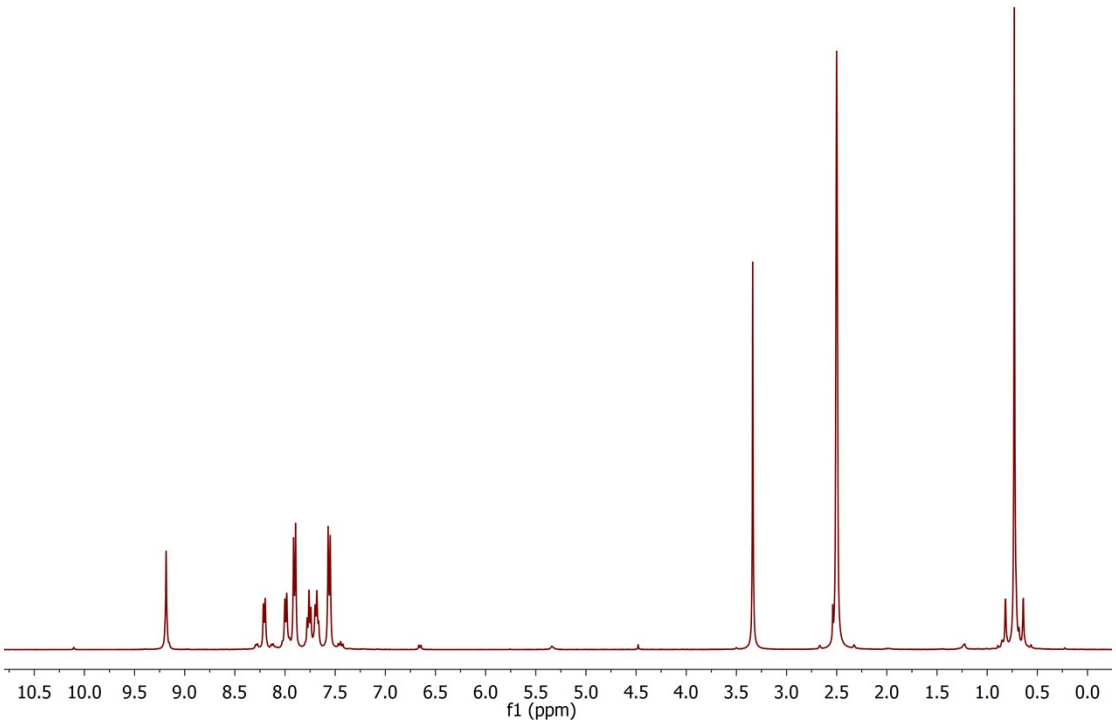

Figure S7. ^{1}H NMR (DMSO-d_6, 20 °C) spectrum of $ClSnMe_2$[2-C_6H_4(4-CH=N-1,1'-$C_6H_4C_6H_4$-4'-N=CH)-2'-C_6H_4]Me_2SnCl (**4**).

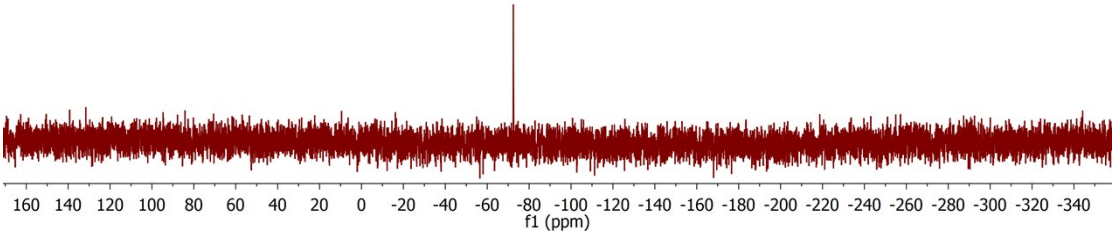

Figure S8. ^{119}Sn NMR (DMSO-d_6, 20 °C) spectrum of $ClSnMe_2$[2-C_6H_4(4-CH=N-1,1'-$C_6H_4C_6H_4$-4'-N=CH)-2'-C_6H_4]Me_2SnCl (**4**).

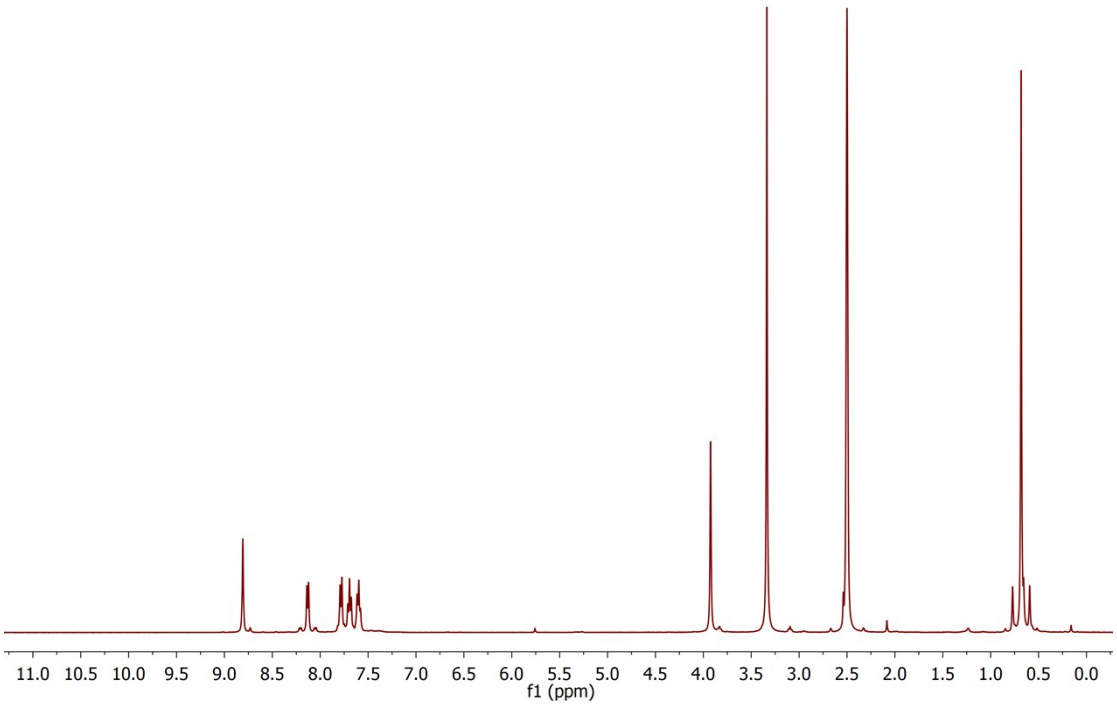

Figure S9. ^{1}H NMR (DMSO-d_6, 20 °C) spectrum of $ClSnMe_2$[2-C_6H_4(CH=NCH_2CH_2N=CH)-2'-C_6H_4]Me_2SnCl (**5**).

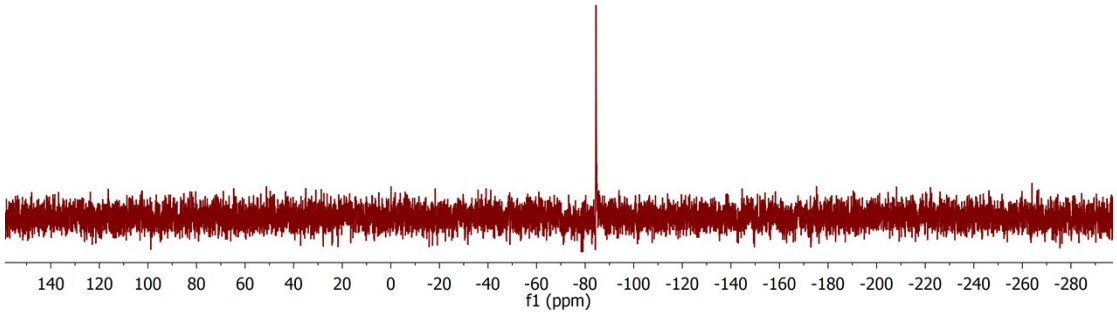

Figure S10. ^{119}Sn NMR (DMSO-d_6, 20 °C) spectrum of $ClSnMe_2$[2-C_6H_4(CH=NCH_2CH_2N=CH)-2'-C_6H_4]Me_2SnCl (**5**).

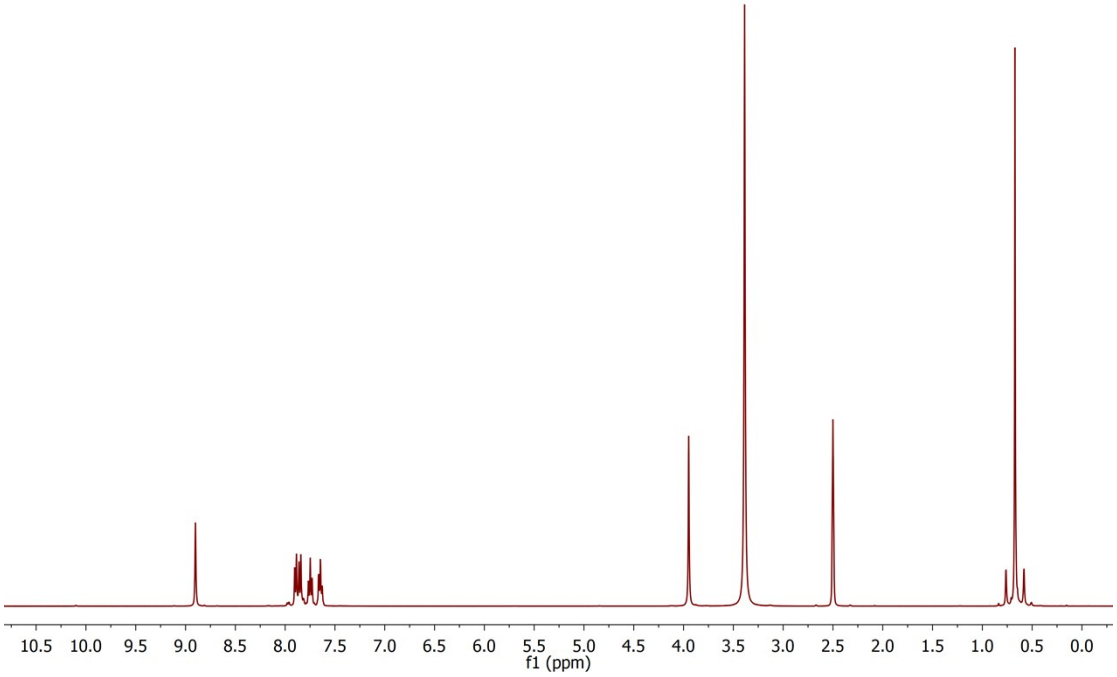

Figure S11. ^{1}H NMR (DMSO-d_6, 20 °C) spectrum of (SCN)SnMe_2[2-C_6H_4(CH=NCH_2CH_2N=CH)-2'-C_6H_4]Me_2Sn(NCS) (**6**)

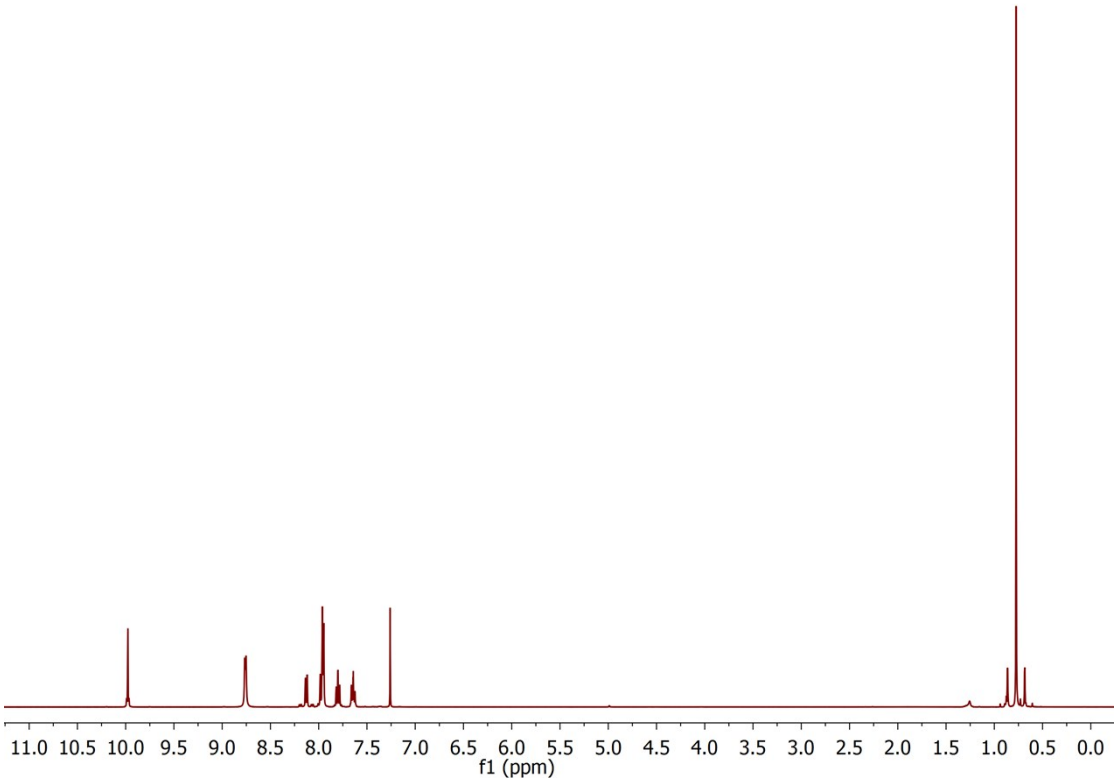

Figure S12. ^{1}H NMR ($CDCl_3$, 20 °C) spectrum of $[2\text{-}(O{=}CH)C_6H_4]Me_2SnO(O)CC_5H_4N\text{-}4$ (**7**).

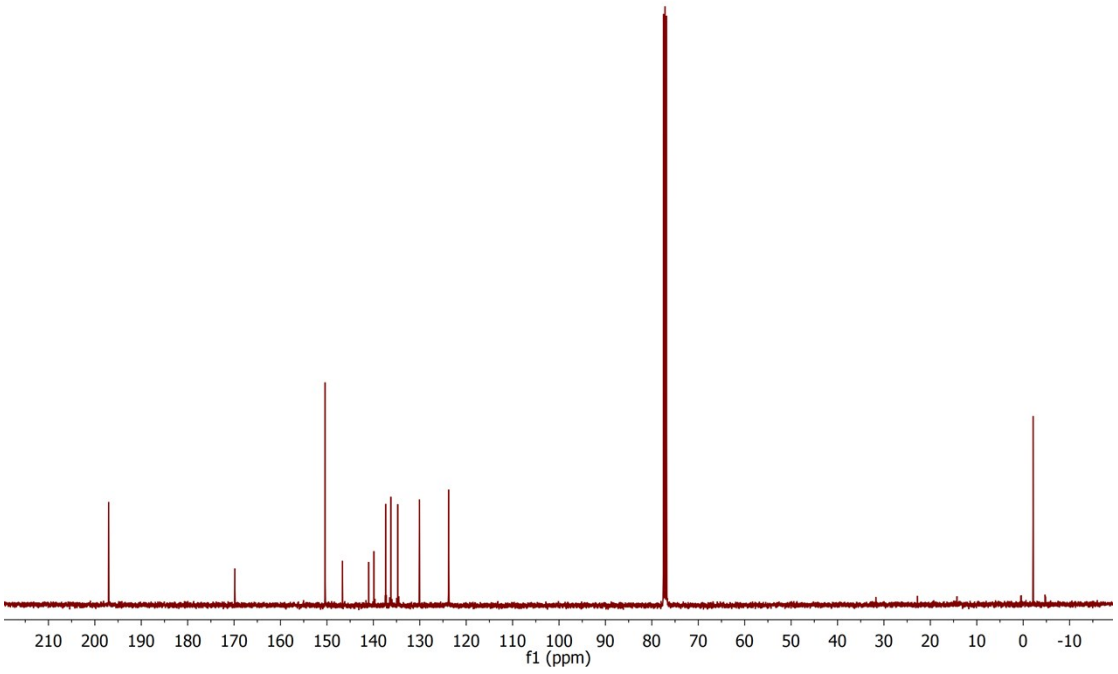

Figure S13. ^{13}C NMR ($CDCl_3$, 20 °C) spectrum of $[2\text{-}(O{=}CH)C_6H_4]Me_2SnO(O)CC_5H_4N\text{-}4$ (**7**).

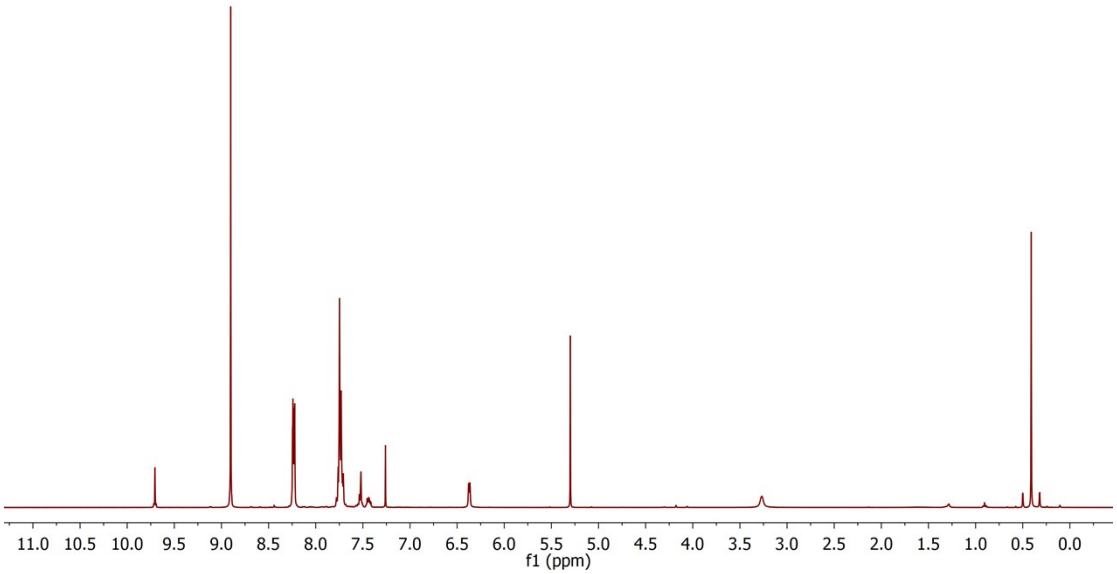

Figure S14. ^{1}H NMR ($CDCl_3$, 20 °C) spectrum of [{2-(O=CH)C_6H_4}Me_2SnO(O)CC_5H_4N-4]ZnTPP (**8**).

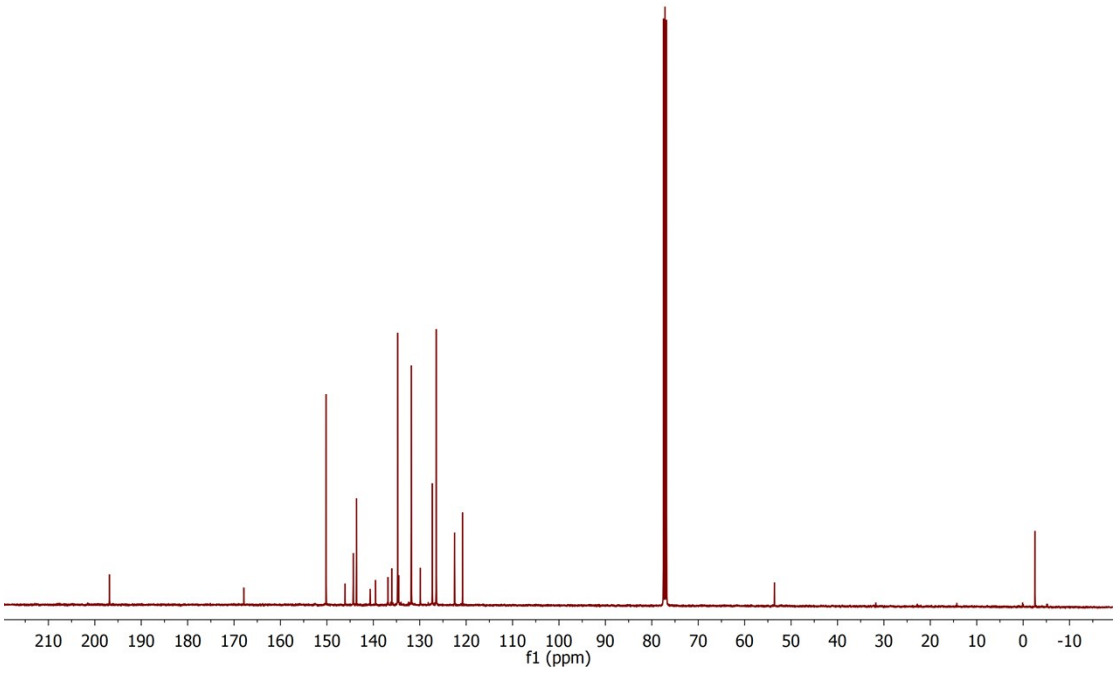

Figure S15. ^{13}C NMR ($CDCl_3$, 20 °C) spectrum of [{2-(O=CH)C_6H_4}Me_2SnO(O)CC_5H_4N-4]ZnTPP (**8**).

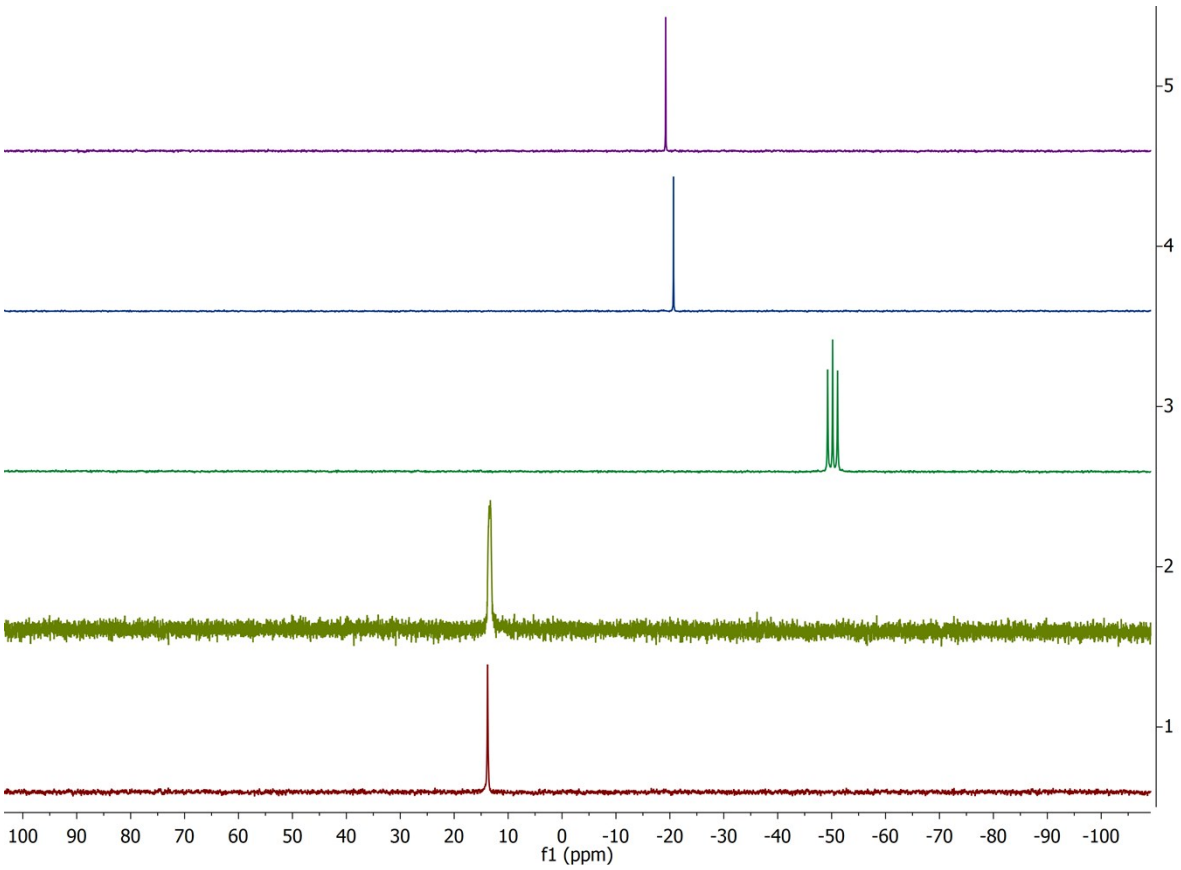

Figure S16. ^{119}Sn NMR ($CDCl_3$, 20 °C) stacked spectra of **1** (spectrum 1), **2** (spectrum 2), **3** (spectrum 3), **7** (spectrum 4) and **8** (spectrum 5).

Table S1. X-ray crystal data and structure refinement for compounds **1**–**3**.

	1	**2**	**3'**	**3''**
Empirical formula	$C_{11}H_{15}ClO_2Sn$	$C_9H_{11}ClOSn$	$C_{10}H_{11}NOSSn$	$C_{10}H_{11}NOSSn$
Formula weight	333.37	289.34	311.95	311.95
Temperature (K)	297(2)	297(2)	297(2)	297(2)
Crystal system	Monoclinic	Orthorhombic	Triclinic	Monoclinic
Space group	$P2_1/n$	*Pbca*	*P*-1	*I2/m*
a (Å)	9.471(3)	12.485(2)	7.3830(16)	13.670(3)
b (Å)	9.488(3)	15.563(3)	11.922(3)	7.4330(15)
c (Å)	15.221(5)	23.473(4)	15.542(3)	24.401(5)
α (º)	90	90	68.185(4)	90
β (º)	106.228(6)	90	80.788(4)	97.77(3)
γ (º)	90	90	81.019(4)	90
Volume (Å^3)	1313.4(8)	4560.7(13)	1246.8(5)	2456.6(9)
Z	4	16	4	8
D_{calc} (g cm^{-3})	1.686	1.685	1.662	1.687
Absorption coefficient (mm^{-1})	2.128	2.432	2.187	2.220
F(000)	656	2240	608	1216
Crystal size (mm)	0.29x0.27x0.23	0.30x0.25x0.23	0.28x0.25x0.10	0.33x0.31x0.30
θ range for data collection (º)	2.283 to 25.007	1.735 to 25.007	1.420 to 25.015	1.621 to 25.003
Reflections collected	9229	41303	11889	11627
Independent reflections	2319 [R_{int} = 0.0321]	4025 [R_{int} = 0.0435]	4378 [R_{int} = 0.0521]	2334 [R_{int} = 0.0319]
Absorption correction	Multi-Scan[1]	Multi-Scan[1]	Multi-Scan[1]	Multi-Scan[1]
Data / restraints / parameters	2319 / 0 / 138	4025 / 0 / 221	4378 / 0 / 257	2334 / 0 / 165
Goodness-of-fit on F^2	1.064	1.284	0.973	1.081
Final *R* indices [$I>2\sigma(I)$]	R_1 = 0.0411 wR_2 = 0.1007	R_1 = 0.0503 wR_2 = 0.0973	R_1 = 0.0443 wR_2 = 0.0835	R_1 = 0.0330 wR_2 = 0.0755
R indices (all data)	R_1 = 0.0520 wR_2 = 0.1069	R_1 = 0.0566 wR_2 = 0.1000	R_1 = 0.0725 wR_2 = 0.0934	R_1 = 0.0393 wR_2 = 0.0787
Largest difference peak and hole (e Å^{-3})	0.90 and −0.70	0.56 and −1.05	0.51 and −0.55	0.52 and −0.40
CCDC No.	1860608	1860615	1860609	1860614

[1] G. M. Sheldrick, *SADABS, Program for area detector adsorption correction*, Institute for Inorganic Chemistry, University of Göttingen, Germany, 1996.

Table S2. X-ray crystal data and structure refinement for compounds **4**-**6** and **8**.

	4	**5**	**6**	**8**
Empirical formula	$C_{30}H_{30}Cl_2N_2Sn_2$	$C_{20}H_{26}Cl_2N_2Sn_2$	$C_{22}H_{26}N_4S_2Sn_2$	$C_{60}H_{45}Cl_2N_5O_3SnZn$
Formula weight	726.84	608.71	647.97	1138.97
Temperature (K)	297(2)	297(2)	297(2)	200(2)
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/n$	C2/c	P21/n
a (Å)	7.340(3)	10.681(2)	12.5737(18)	21.938(4)
b (Å)	12.824(5)	9.7590(19)	18.303(3)	11.1466(18)
c (Å)	15.719(5)	11.374(2)	12.8154(18)	21.982(4)
α (º)	90	90	90	90
β (º)	96.371(6)	106.171(3)	92.033(3)	95.914(3)
γ (º)	90	90	90	90
Volume (Å^3)	1470.5(9)	1138.6(4)	2947.5(7)	5346.8(15)
Z	2	2	4	4
D_{calc} (g cm^{-3})	1.642	1.758	1.460	1.415
Absorption coefficient (mm^{-1})	1.901	2.435	1.850	1.065
F(000)	716	588	1272	2312
Crystal size (mm)	0.21x0.19x0.18	0.15x0.12x0.05	0.31x0.28x0.26	0.40x0.25x0.20
θ range for data collection (º)	2.608 to 25.010	1.864 to 25.005	2.492 to 25.006	1.866 to 25.000
Reflections collected	12709	10741	13802	26981
Independent reflections	2565	2007	2595	9376
	[R_{int} = 0.0451]	[R_{int} = 0.0570]	[R_{int} = 0.0431]	[R_{int} = 0.0910]
Absorption correction	Multi-Scan[1]	Multi-Scan[1]	Multi-Scan[1]	Multi-Scan[1]
Data / restraints / parameters	2565 / 0 / 165	2007 / 0 / 121	2595 / 0 / 139	9376 / 0 / 652
Goodness-of-fit on F^2	1.192	1.181	1.051	0.785
Final R indices [I>2σ(I)]	R_1 = 0.0472	R_1 = 0.0600	R_1 = 0.0385	R_1 = 0.0656
	wR_2 = 0.1038	wR_2 = 0.1567	wR_2 = 0.0812	wR_2 = 0.1576
R indices (all data)	R_1 = 0.0564	R_1 = 0.0625	R_1 = 0.0488	R_1 = 0.1096
	wR_2 = 0.1082	wR_2 = 0.1587	wR_2 = 0.0857	wR_2 = 0.1902
Largest difference peak and hole (e Å^{-3})	0.63 and −0.55	3.26 and −0.77	0.53 and −0.29	0.71 and −0.87
CCDC No.	1860611	1860610	1860612	1860613

[1] G. M. Sheldrick, *SADABS, Program for area detector adsorption correction*, Institute for Inorganic Chemistry, University of Göttingen, Germany, 1996.

Table S3. Selected bond distances (Å) and angles (°) for compounds **2b**, **3′b** and **3′′b**.

2b		**3′b**		**3′′b**[a]	
Sn(2)–C(10)	2.141(6)	Sn(2)–C(11)	2.136(6)	Sn(2)–C(11)	2.122(6)
Sn(2)–C(17)	2.107(7)	Sn(2)–C(18)	2.111(6)	Sn(2)–C(18)	2.107(4)
Sn(2)–C(18)	2.113(7)	Sn(2)–C(19)	2.107(5)	Sn(2)–C(18a)^{i}	2.107(4)
Sn(2)–Cl(2)	2.4418(19)				
Sn(2)–O(2)	2.491(4)	Sn(2)–O(1)	2.451(4)	Sn(2)–O(2)	2.442(4)
		Sn(2)–N(2)	2.180(6)	Sn(2)–N(2)	2.161(6)
C(16)–O(2)	1.215(7)	C(17)–O(2)	1.217(7)	C(17)–O(2)	1.206(8)
		C(20)–N(2)	1.142(7)	C(19)–N(2)	1.162(8)
		C(20)–S(2)	1.586(7)	C(19)–S(2)	1.594(7)
Cl(2)–Sn(2)–O(2)	170.33(12)	N(2)–Sn(2)–O(2)	169.27(18)	N(2)–Sn(2)–O(2)	169.20(19)
C(10)–Sn(2)–C(17)	119.8(3)	C(11)–Sn(2)–C(18)	118.0(2)	C(11)–Sn(2)–C(18)	118.78(12)
C(10)–Sn(2)–C(18)	113.5(3)	C(11)–Sn(2)–C(19)	117.5(2)	C(11)–Sn(2)–C(18a)^{i}	118.78(12)
C(17)–Sn(2)–C(18)	120.7(3)	C(18)–Sn(2)–C(19)	121.1(2)	C(18)–Sn(2)–C(18a)^{i}	117.7(2)
Cl(2)–Sn(2)–C(10)	96.86(16)	N(2)–Sn(2)–C(1)	94.8(2)	N(2)–Sn(2)–C(11)	95.7(2)
Cl(2)–Sn(2)–C(17)	98.4(3)	N(2)–Sn(2)–C(18)	96.7(2)	N(2)–Sn(2)–C(18)	98.04(15)
Cl(2)–Sn(2)–C(18)	99.3(3)	N(2)–Sn(2)–C(19)	97.0(2)	N(2)–Sn(2)–C(18a)^{i}	98.04(15)
O(2)–Sn(2)–C(10)	73.47(18)	O(2)–Sn(2)–C(11)	74.42(19)	O(2)–Sn(2)–C(11)	73.52(19)
O(2)–Sn(2)–C(17)	87.0(3)	O(2)–Sn(2)–C(18)	88.4(2)	O(2)–Sn(2)–C(18)	87.47(13)
O(2)–Sn(2)–C(18)	84.7(3)	O(2)–Sn(2)–C(19)	88.3(2)	O(2)–Sn(2)–C(18a)^{i}	87.47(13)
C(11)–C(16)–O(2)	122.7(6)	C(12)–C(17)–O(2)	124.4(6)	C(12)–C(17)–O(2)	124.5(6)
C(16)–O(2)–Sn(2)	108.3(4)	C(17)–O(2)–Sn(2)	108.2(4)	C(17)–O(2)–Sn(2)	108.2(4)
		N(2)–C(20)–S(2)	178.8(7)	N(2)–C(19)–S(2)	177.7(6)
		Sn(2)–N(2)–C(20)	161.4(6)	Sn(2)–N(2)–C(19)	175.7(6)

[a] Symmetry codes: (i) *x*, –*y*, *z*, for **3′′b**.

- the crystal contains a 1:1 mixture of $pR_{O(1)}$-$R_{C(7)}$-**1** and $pS_{O(1)}$-$S_{C(7)}$-**1**

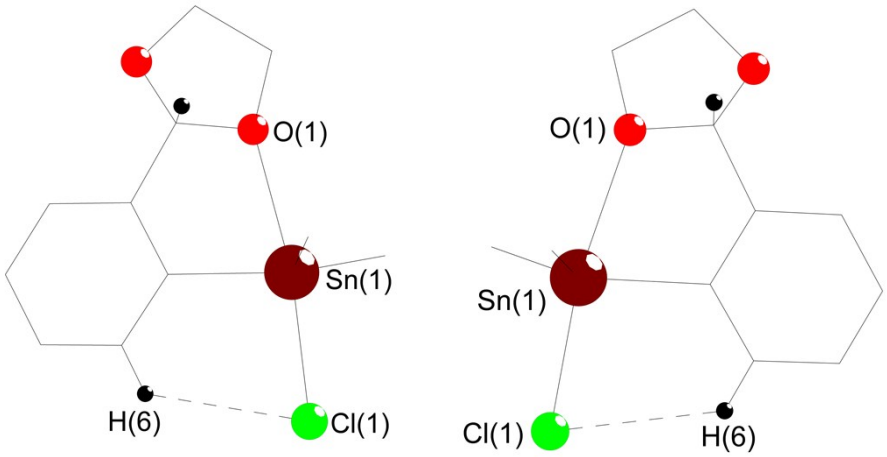

Figure S17. Molecular structure of $pR_{O(1)}$-$R_{C(7)}$-**1** isomer (*left*) and $pS_{O(1)}$-$S_{C(7)}$-**1** isomer (*right*) in the crystal of **1**, showing the intramolecular chlorine-hydrogen contacts (only methine hydrogens and hydrogen atoms involved in intramolecular contacts are shown).

- intramolecular distance Cl(1)···$H(6)_{aryl}$ 2.77 Å $\sum r_{vdW}$(Cl,H) 3.01 Å

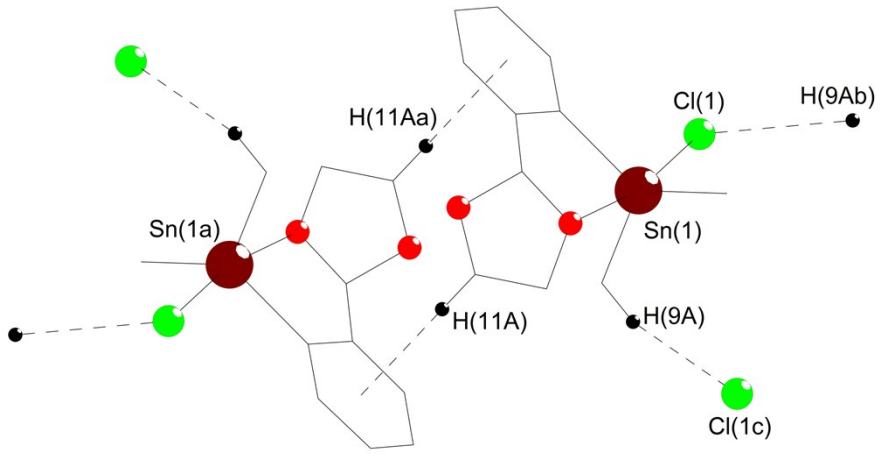

Figure S18. View of a dimer association of $pR_{O(1)}$-$R_{C(7)}$-**1** and $pS_{O(1)}$-$S_{C(7)}$-**1** isomers isomers based on intermolecular C–H···π ($Ph_{centroid}$) contacts in the crystal of **1** (only hydrogen atoms involved in intermolecular contacts are shown) [symmetry equivalent atoms (*1–x, 1–y, 1–z*), (*1.5–x, –0.5+y, 0.5–z*) and (*1.5–x, 0.5+y, 0.5–z*) are given by "a", "b" and "c", respectively].

- intermolecular distance Cl(1)···$H(9Ab)_{methyl}$ 2.90 Å
  $C(11a)–H(9Aa)_{methylene}$···$Ph_{centroid}${C(1)-C(6)} 2.79 Å
  $\gamma = 7.9°$

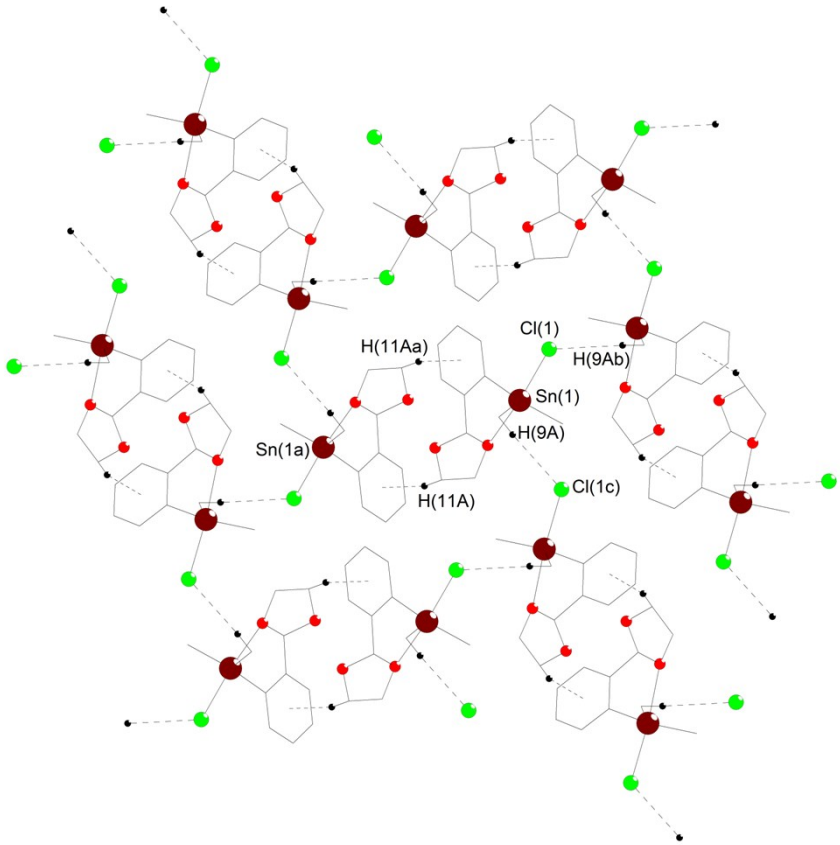

Figure S19. View of a honeycomb-type layer based on intermolecular C–H···π ($Ph_{centroid}$) and chlorine-hydrogen contacts in the crystal of **1** (only hydrogen atoms involved in intermolecular contacts are shown) [symmetry equivalent atoms (*1–x, 1–y, 1–z*), (*1.5–x, –0.5+y, 0.5–z*) and (*1.5–x, 0.5+y, 0.5–z*) are given by "a", "b" and "c", respectively].

- no further contacts between parallel layers.

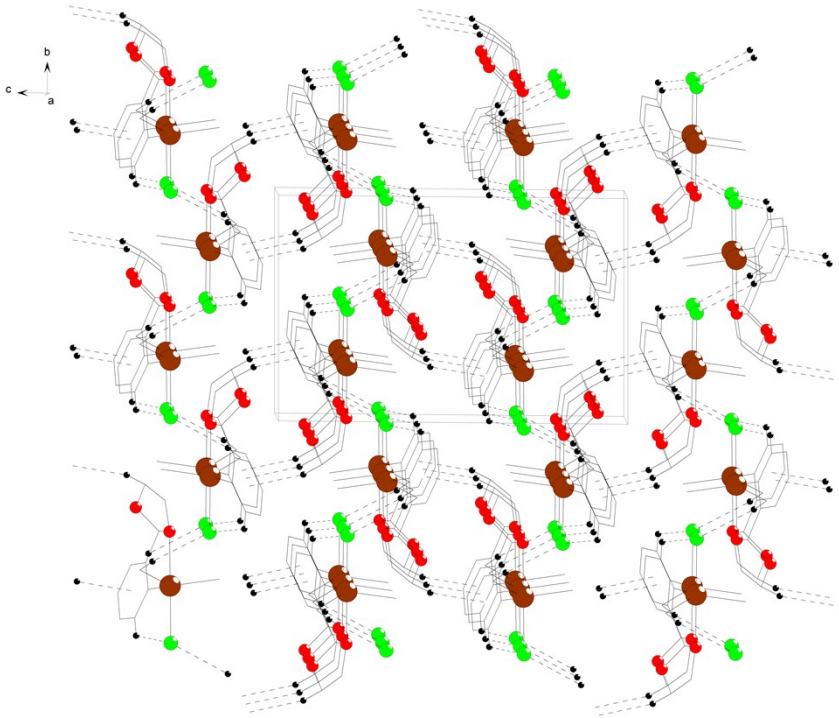

Figure S20. View along *a* axis of the layered structure in the crystal of **1** (only hydrogen atoms involved in intra- and intermolecular contacts are shown).

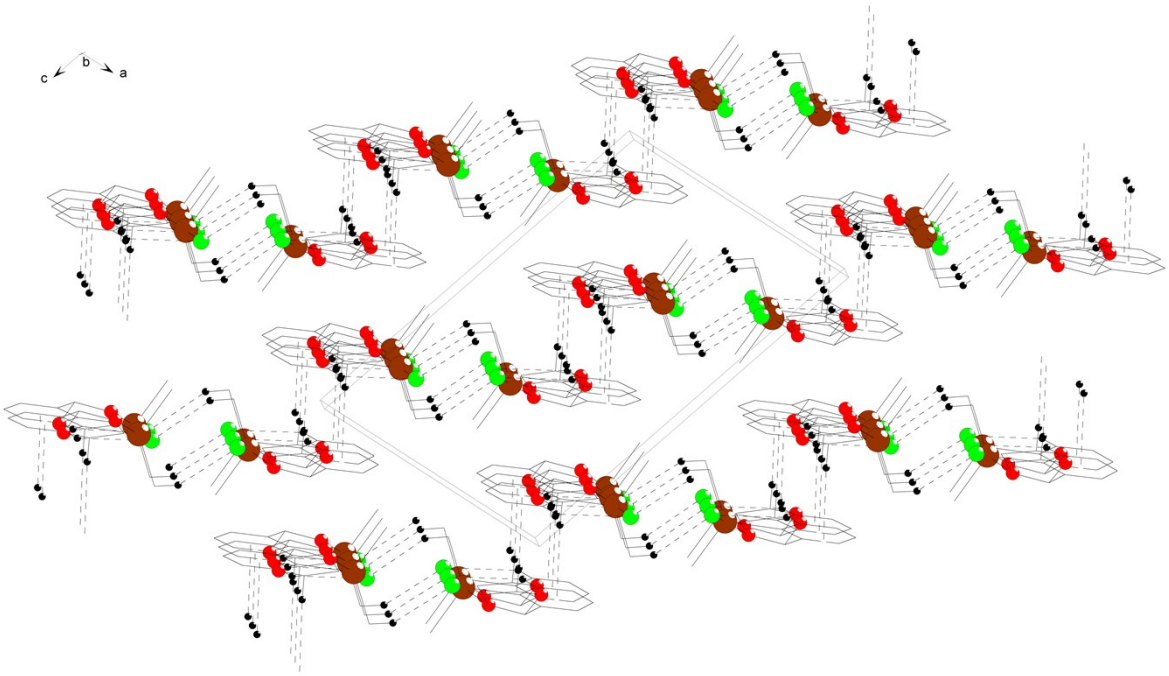

Figure S21. Packing of **1** viewed along *b* axis, showing the arrangement of the layers (only hydrogen atoms involved in intra- and intermolecular contacts are shown).

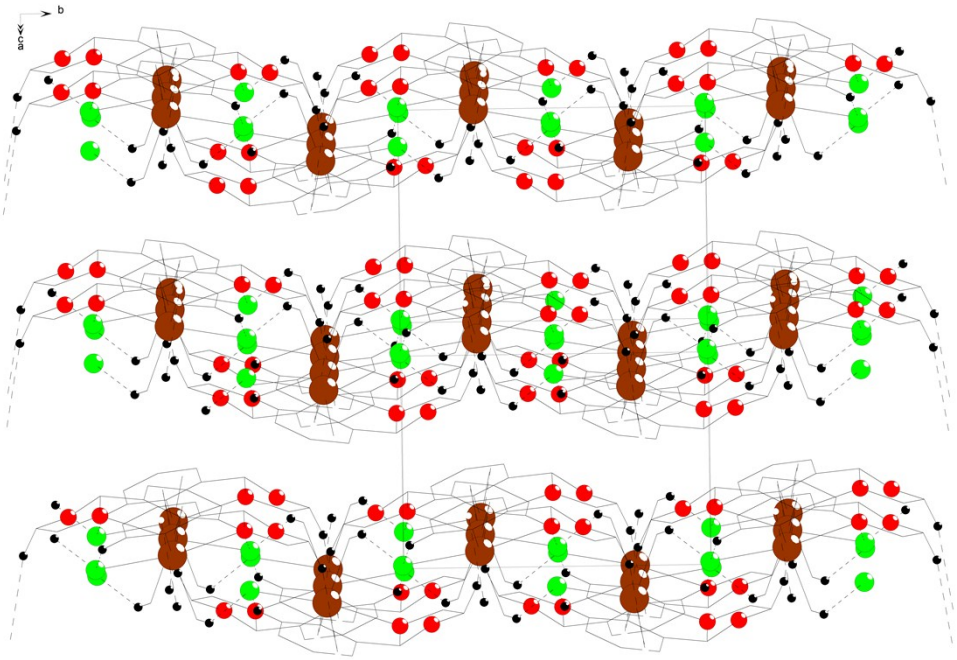

Figure S22. Packing of **1** viewed perpendicular to the bisecting line of *a* and *c* axis and also *b* axis, respectively, showing the arrangement of the layers (only hydrogen atoms involved in intra- and intermolecular contacts are shown).

- the crystal contains two independent molecules

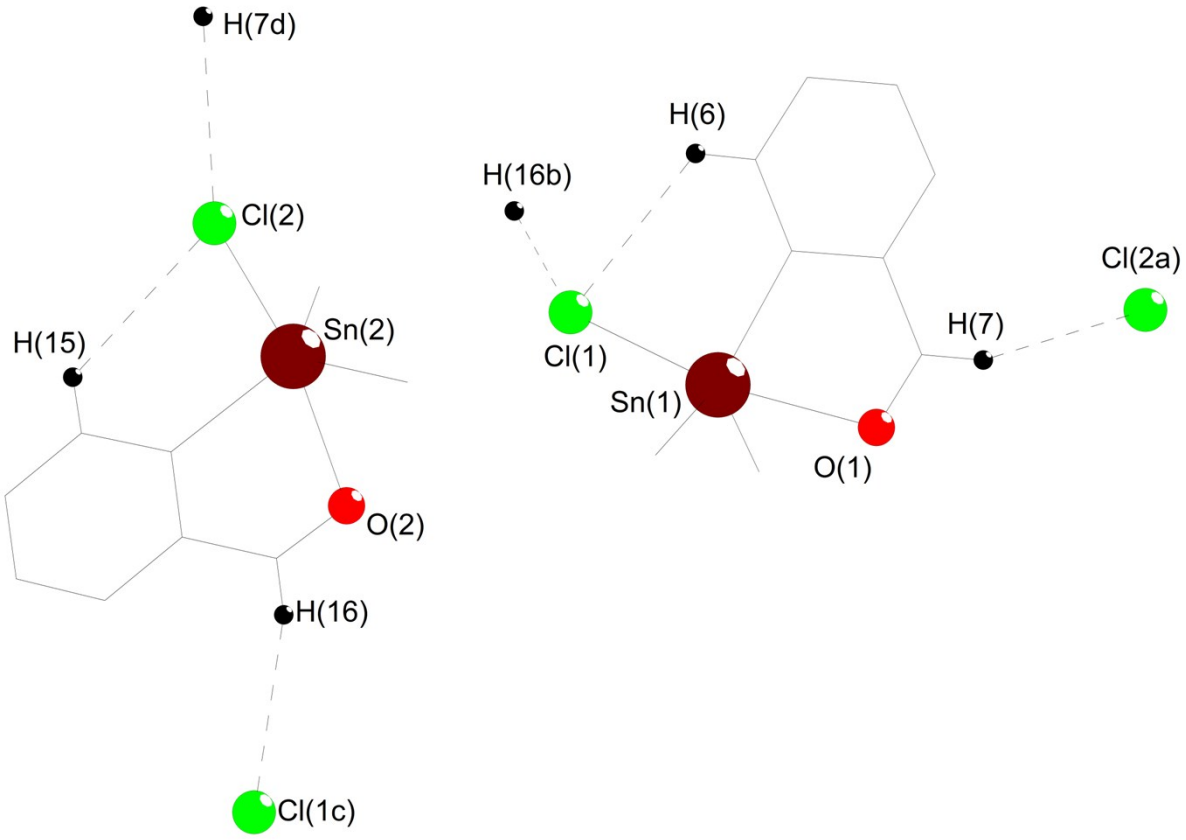

Figure S23. Molecular structure of the two independent molecules in the crystal of **2**, showing the intra- and intermolecular chlorine-hydrogen contacts (only carbonyl hydrogens and hydrogen atoms involved in contacts are shown) [symmetry equivalent atoms (*x, 0.5–y, –0.5+z*), (*1.5–x, –0.5+y, z*), (*1.5–x, 0.5+y, z*) and (*x, 0.5–y, 0.5+z*) are given by "a", "b", "c" and "d" respectively].

-	intramolecular distance	Cl(1)···H(6)$_{aryl}$ 2.84 Å	$\sum r_{vdW}$(Cl,H) 3.01 Å
		Cl(2)···H(15)$_{aryl}$ 2.89 Å	
-	intermolecular distance	C1(1)···H(16b)$_{carbonyl}$ 2.85 Å	
		Cl(2)···H(7d)$_{carbonyl}$ 2.91 Å	

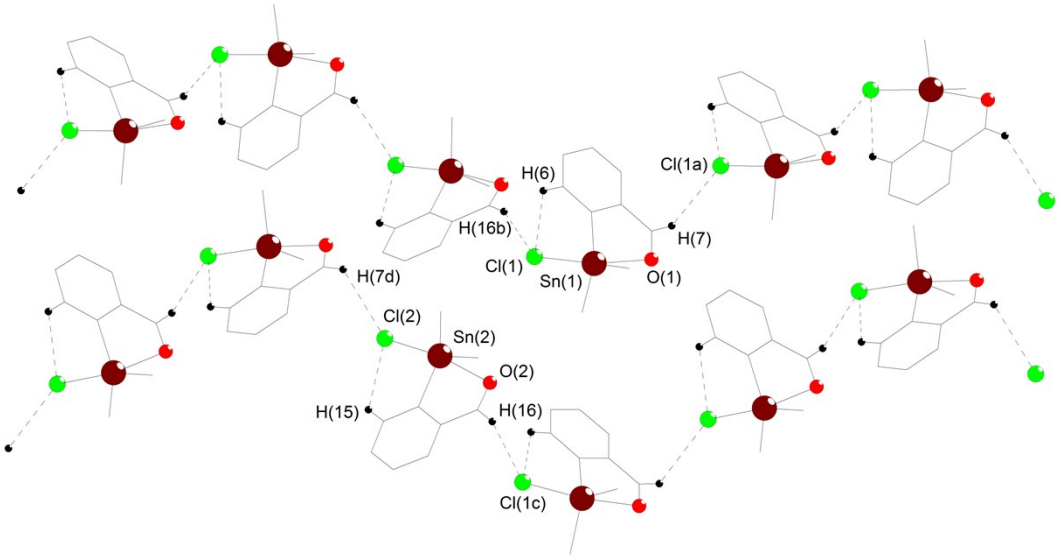

Figure S24. View along *a* axis of the M (uper) and P (lower) helicoidal polymers based on intermolecular chlorine-hydrogen contacts in the crystal of **2** (only carbonyl hydrogens and hydrogen atoms involved in contacts are shown) [symmetry equivalent atoms (*x, 0.5–y, –0.5+z*), (*1.5–x, –0.5+y, z*), (*1.5–x, 0.5+y, z*) and (*x, 0.5–y, 0.5+z*) are given by "a", "b", "c" and "d" respectively].

- no further contacts between different polymers.

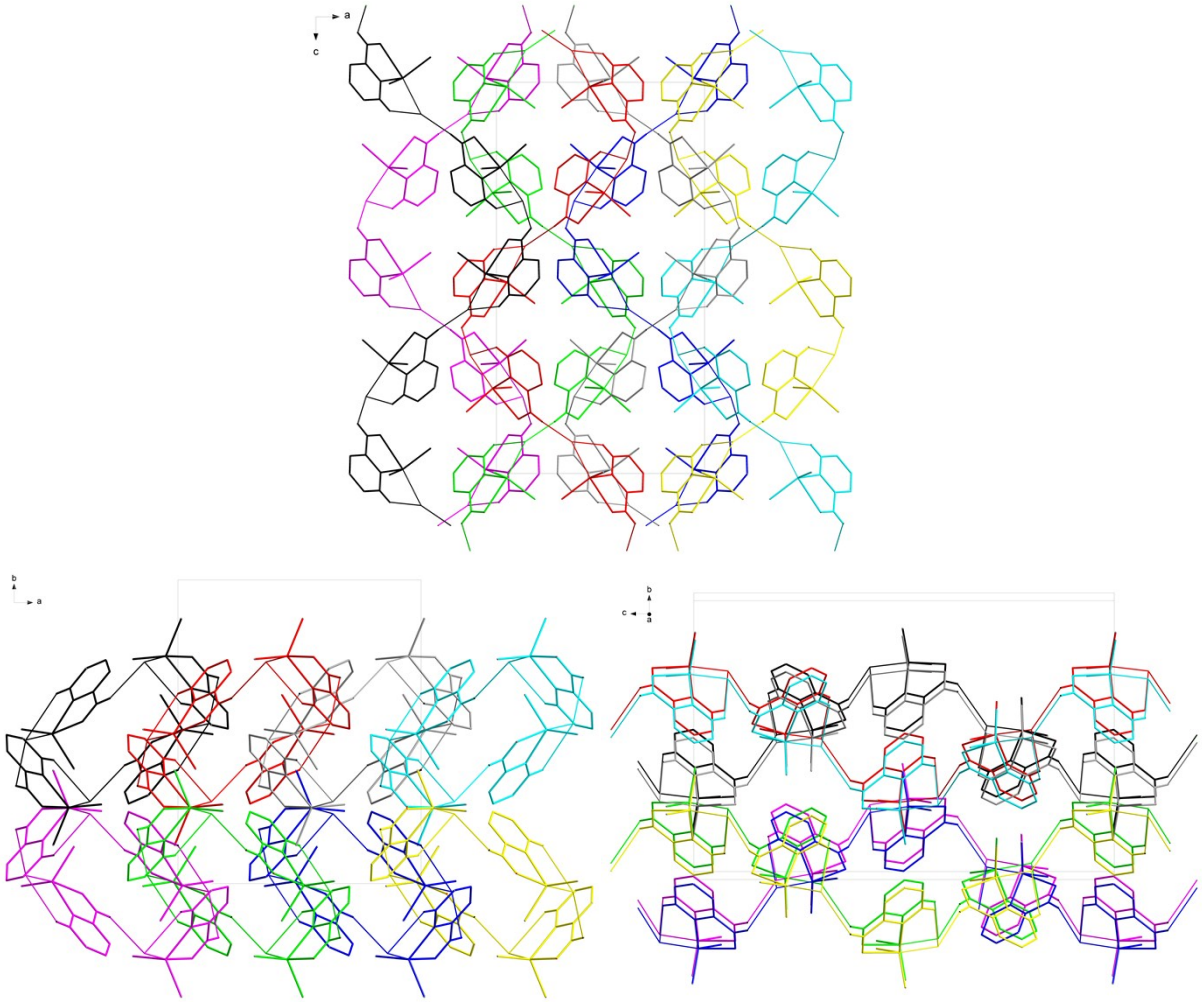

Figure S25. View along *b* (top), *c* (bottom-left) and *a* (bottom-right) axis of the arrangement of the helicoidal polymers based on chlorine-hydrogen contacts in the crystal of **2** (only hydrogen atoms involved in intermolecular contacts are shown; each polymer was drawn with a different colour).

- 3'- the crystal contains two independent molecules

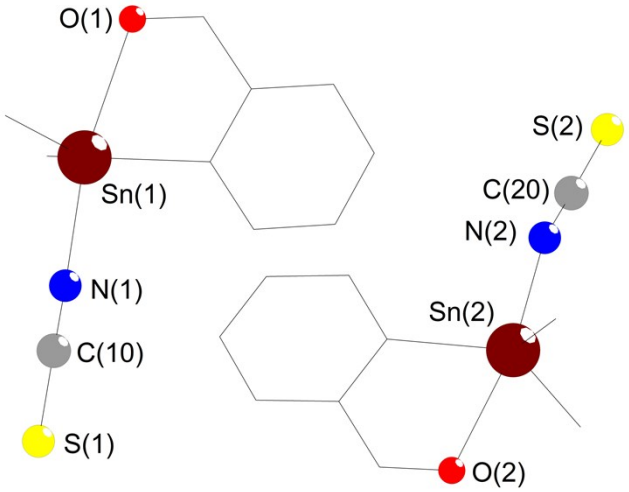

Figure S26. Molecular structure of the two independent molecules in the crystal of **3'**, (hydrogen atoms are omitted for clarity).

- no further contacts between different molecules.

- 3''- the crystal contains two independent molecules laying on a mirror plane

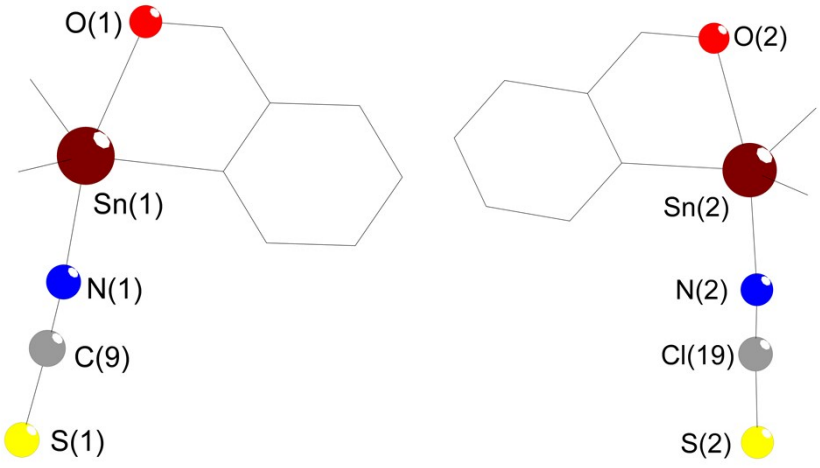

Figure S27. Molecular structure of the two independent molecules in the crystal of **3''**, (hydrogen atoms are omitted for clarity).

- no further contacts between different molecules.

ClSnMe$_2$[2-C$_6$H$_4$(4-CH=N-1,1'-C$_6$H$_4$C$_6$H$_4$-4'-N=CH)-2'-C$_6$H$_4$]Me$_2$SnCl (4)

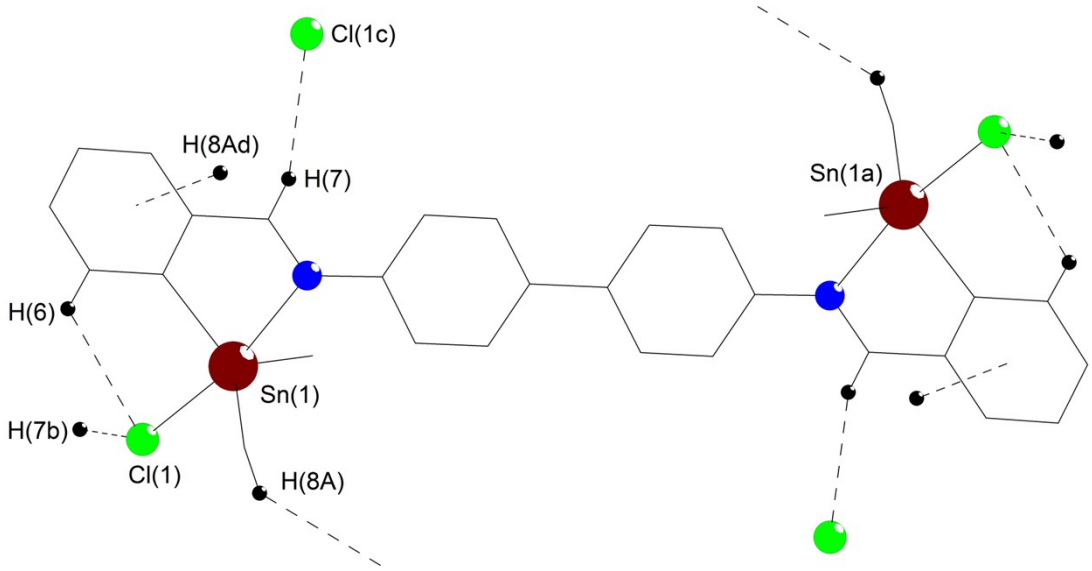

Figure S28. View of the chlorine-hydrogen and C–H···π (Ph$_{centroid}$) contacts in the crystal of **4** (only hydrogen atoms involved in intra- and intermolecular contacts are shown) [symmetry equivalent atoms (*2–x, 1–y, 2–z*), (*–0.5+x, 1.5–y, 0.5+z*), (*0.5+x, 1.5–y, 0.5+z*) and (*0.5–x, 0.5+y, 1.5–z*) are given by "a", "b", "c" and "d" respectively].

- intramolecular distance Cl(1)···H(6)$_{aryl}$ 2.84 Å $\sum r_{vdW}$(Cl,H) 3.01 Å

- intermolecular distance Cl(1)···H(7b)$_{imine}$ 2.82 Å
  C(8d)–H(8Ad)$_{methyl}$···Ph$_{centroid}${C(1)-C(6)} 3.04 Å
  γ = 20.7°

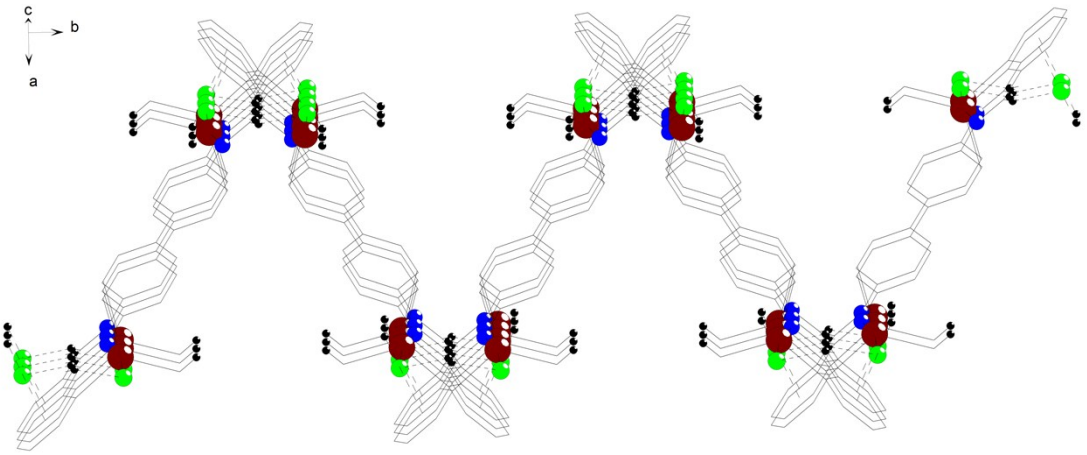

Figure S29. View along *c* axis of a zig-zag layer based on chlorine-hydrogen contacts in the crystal of **4** (only hydrogen atoms involved in intermolecular contacts are shown).

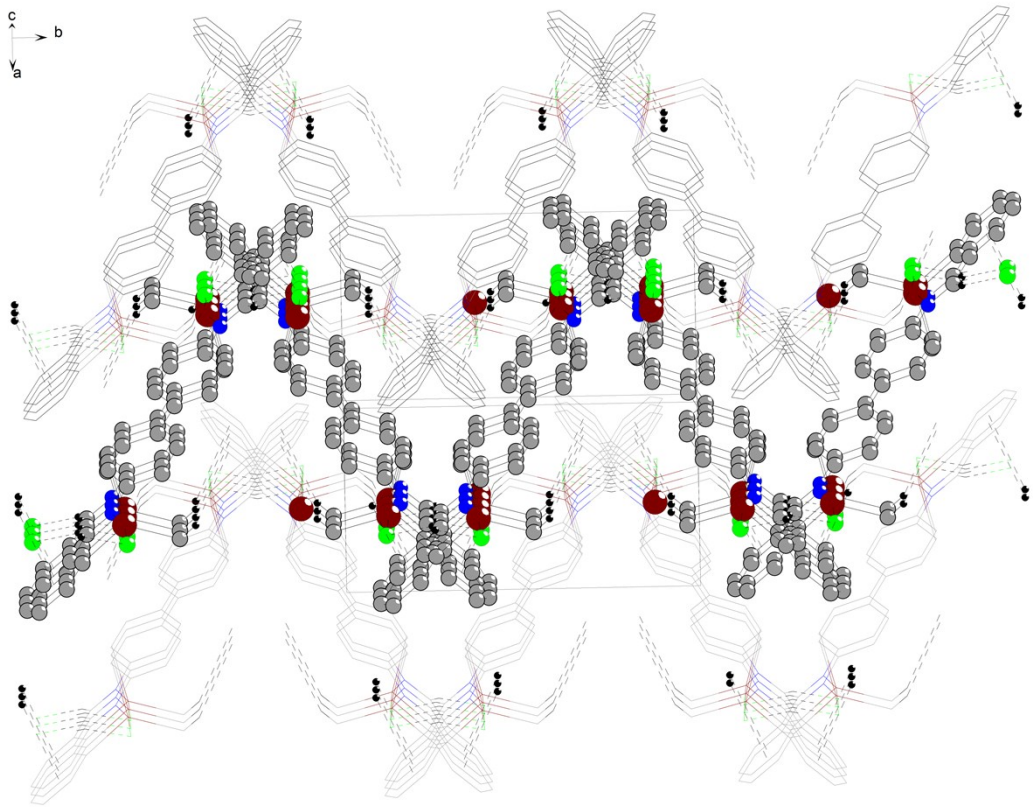

Figure S30. Packing of **4** along *c* axis showing the 3D architecture based on zig-zag layers connected by C–H···π ($Ph_{centroid}$) interactions (only hydrogen atoms involved in intermolecular contacts are shown).

$ClSnMe_2[C_6H_4(CH{=}NCH_2CH_2N{=}CH)C_6H_4]Me_2SnCl$ (5)

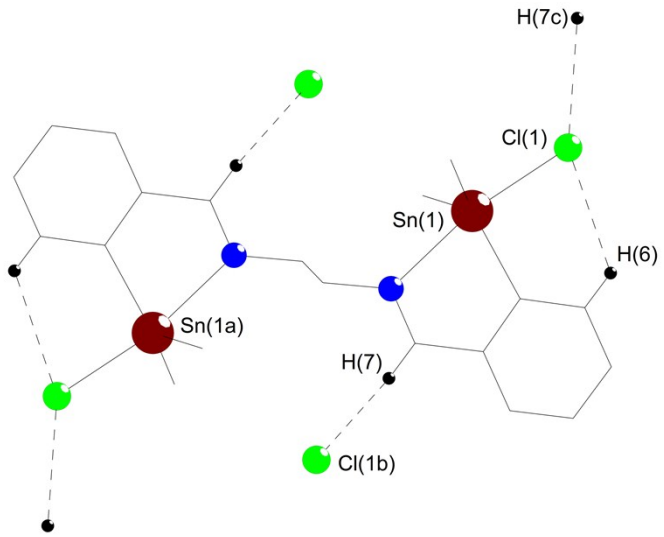

Figure S31. Molecular structure of **5**, showing the intra- and intermolecular chlorine-hydrogen contacts (only hydrogen atoms involved in contacts are shown) [symmetry equivalent atoms (*–x,–y, 2–z*), (*–0.5+x, 0.5–y, 0.5+z*) and (*0.5+x, 0.5–y, –0.5+z*) (are given by "a", "b" and "c", respectively].

- intramolecular distance $Cl(1)\cdots H(6)_{aryl}$ 2.86 Å $\sum r_{vdW}(Cl,H)$ 3.01 Å
- intermolecular distance $Cl(1)\cdots H(7c)_{imine}$ 2.86 Å

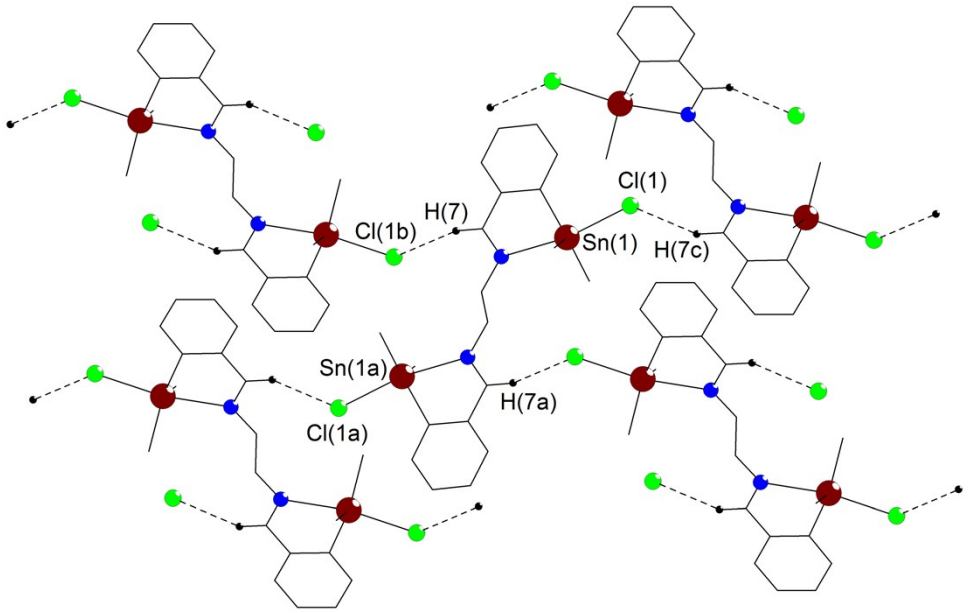

Figure S32. View of a layer based on intermolecular chlorine-hydrogen contacts in the crystal of **5** (only hydrogen atoms involved in intermolecular contacts are shown) [symmetry equivalent atoms (*–x, –y, 2–z*), (*–0.5+x, 0.5–y, 0.5+z*), and (*0.5+x, 0.5–y, –0.5+z*) are given by "a", "b" and "c", respectively].

- no further contacts between different layers.

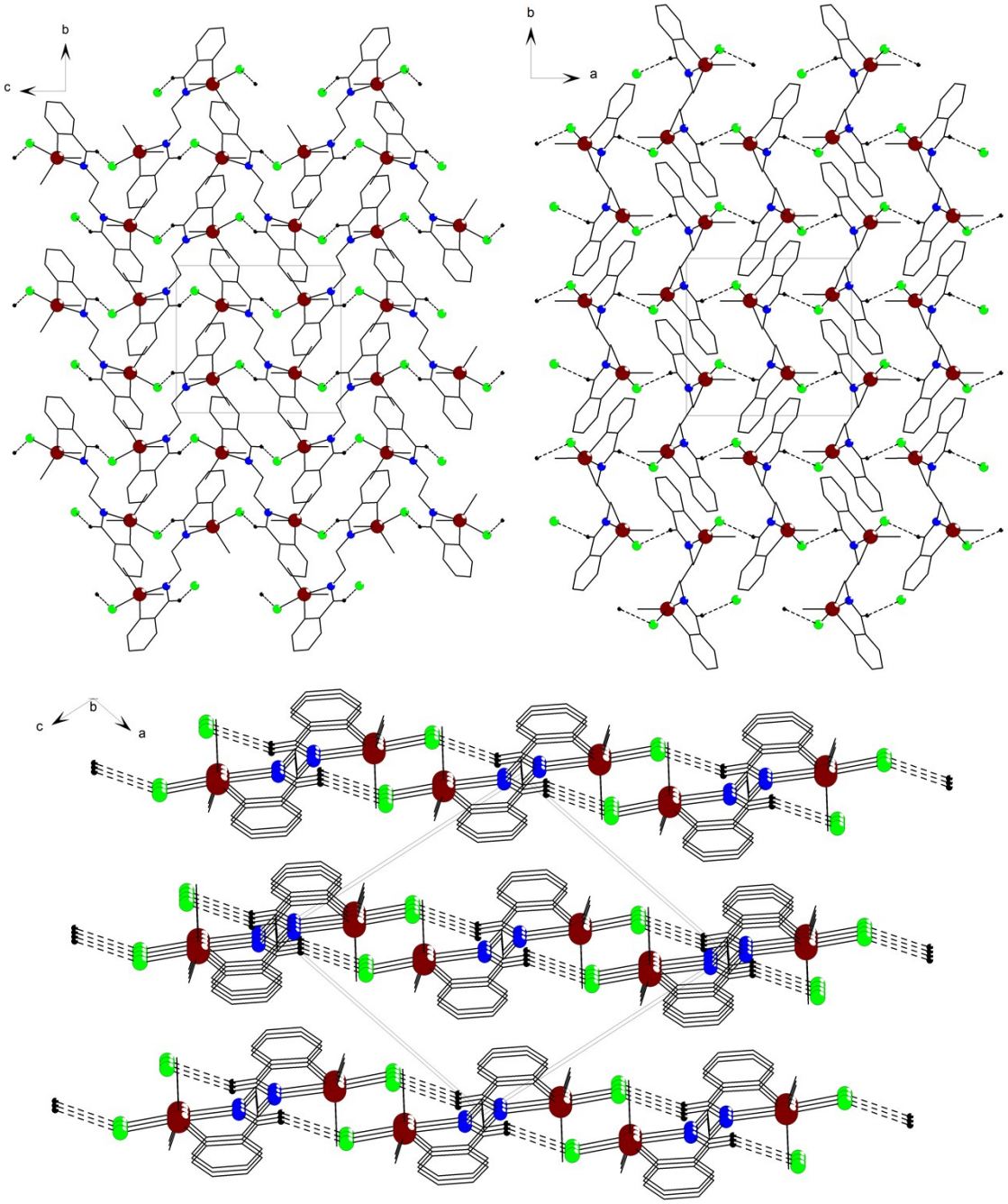

Figure S33. Packing of **5** along the *a*, *b* and *c* axis showing the arrangement of the supramolecular layers in crystal.

(SCN)SnMe$_2$[2-C$_6$H$_4$(CH=NCH$_2$CH$_2$N=CH)-2'-C$_6$H$_4$]Me$_2$Sn(NCS) (6)

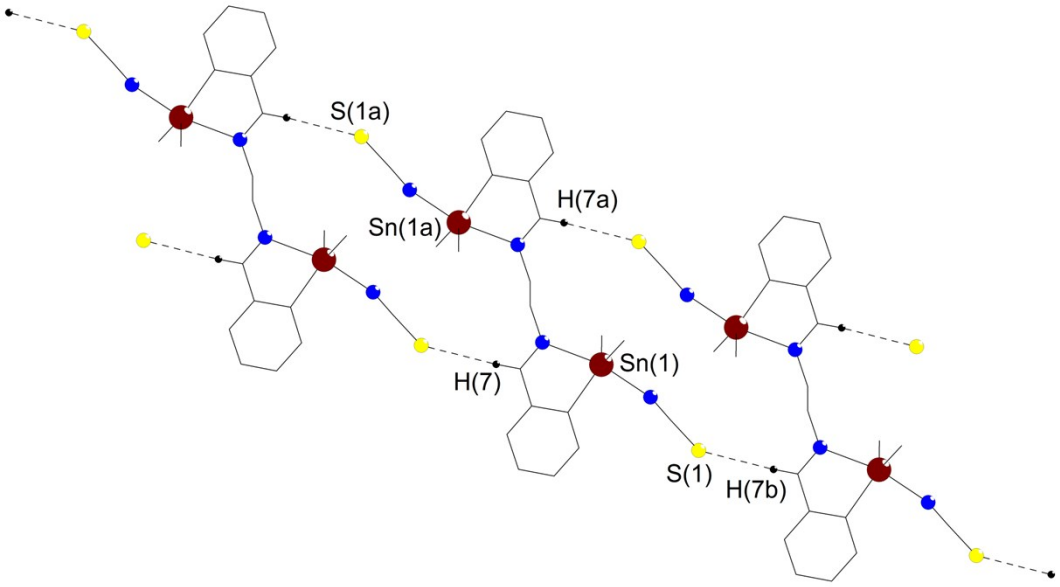

Figure S34. View of the ribbon-like polymer based on sulfur-hydrogen contacts in the crystal of **6** (only hydrogen atoms involved in intermolecular contacts are shown) [symmetry equivalent atoms (*0.5–x, 1.5–y, 2–z*) and (*0.5+x, –0.5+y, z*) are given by "a" and "b", respectively].

- intermolecular distance S(1)···H(7b)$_{imine}$ 2.84 Å $\sum r_{vdW}$(S,H) 3.0 Å
- no contacts between different chains.

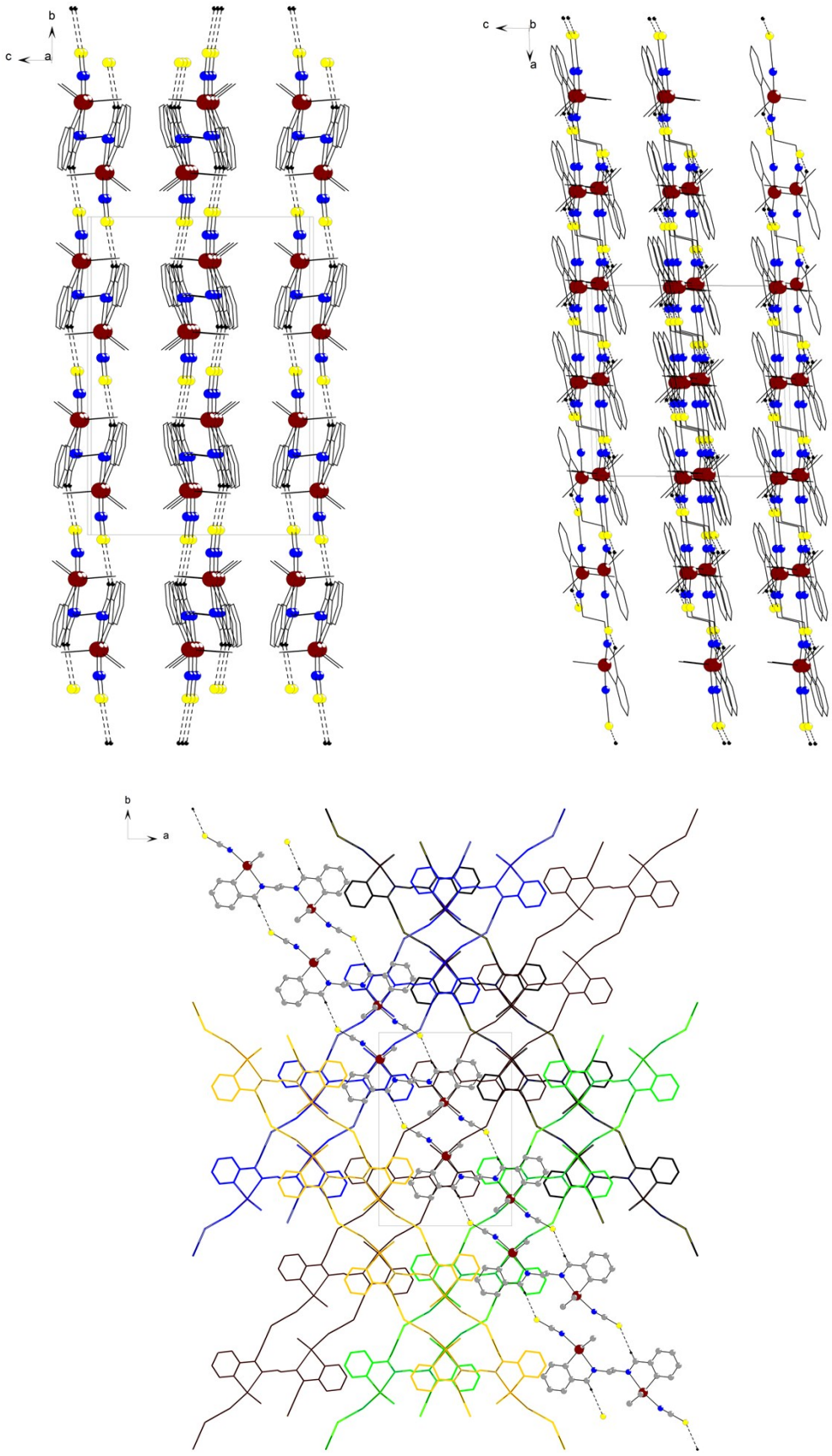

Figure S35. Packing of **6** along the *a*, *b* and *c* axis in crystal.

[{2-(O=CH)C_6H_4}Me_2Sn-OOC-(4-C_5H_4N)]ZnTPP (8)

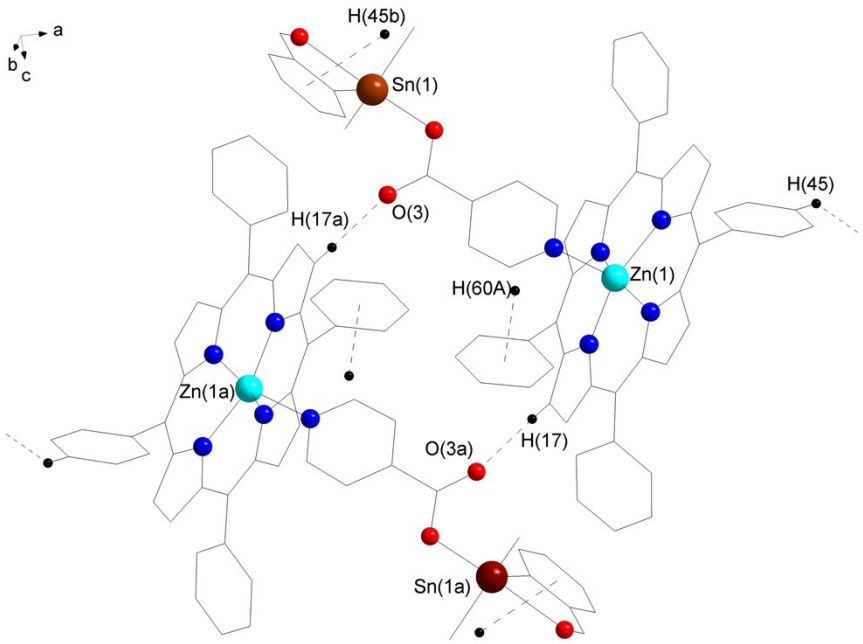

Figure S36. View of the dimer association based on oxygen-hydrogen contacts and the C–H···π ($Ph_{centroid}$) contacts with other dimers in the crystal of **8** (only hydrogen atoms involved in intermolecular contacts are shown) [symmetry equivalent atoms (*1–x, 2–y, 1–z*) and (*–1.5–x, –0.5+y, 0.5–z*)) are given by "a", and "b", respectively].

- intermolecular distance $O(3)\cdots H(17a)_{TPP}$ 2.44 Å $\sum r_{vdW}(O,H)$ 2.6 Å
  $C(45b)–H(45b)_{Ph\text{-}TPP}\cdots Ph_{centroid}\{C(1)\text{-}C(6)\}$ 2.79 Å
  γ = 15.9°
  $C(60)–H(60A)_{dichloromethane}\cdots Ph_{centroid}\{C(54)\text{-}C(59)\}$ 2.81 Å
  γ = 11.7°

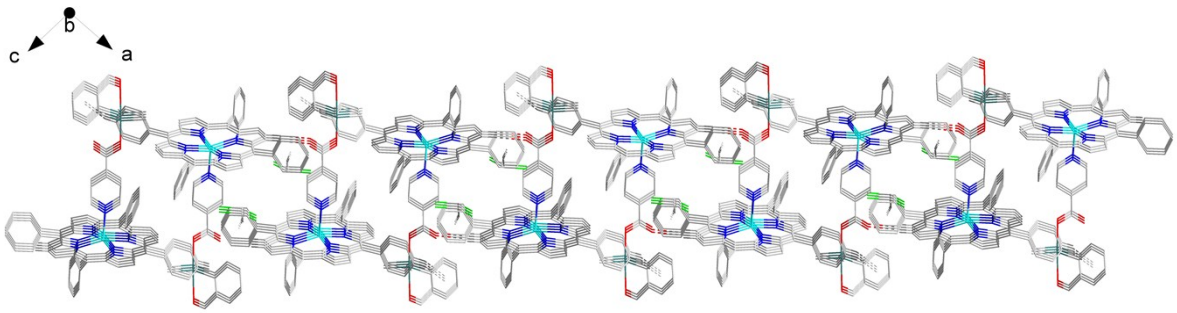

Figure S37. View of the double layer based on oxygen-hydrogen and C–H···π ($Ph_{centroid}$) contacts in the crystal of **8** (only hydrogen atoms involved in intermolecular contacts are shown).