

## Supplementary Material

### Synthesis, Characterization, and Theoretical Studies of *cis*-Dichloridobis(8-quinolinethiolato)tin(IV) and bis(8-Sulfanylquinolinium) Hexachloridostannate(IV) Derivatives

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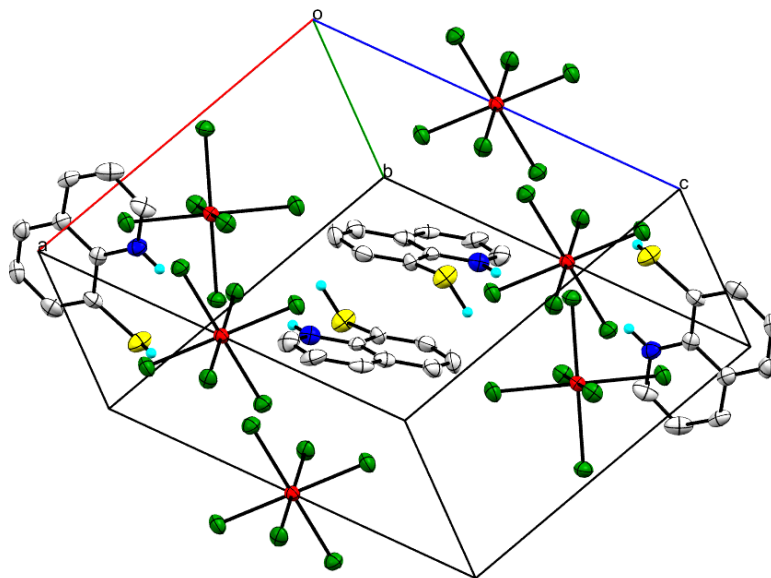
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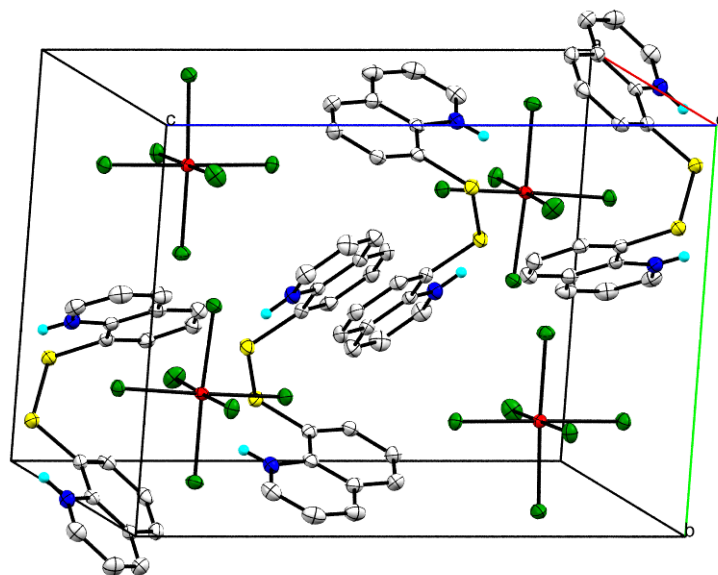
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**Figure S1.** Packing Diagram of 2.



**Figure S2.** Packing Diagram of 4.

**Table S1.** Refinement details for the X-ray structures of 2-4

Compound	2	3m	3t	4
Crystal system	Monoclinic	Monoclinic	Triclinic	Monoclinic
Space group	<i>P2<sub>1</sub>/n</i>	<i>C2/c</i>	<i>P-1</i>	<i>P2<sub>1</sub>/n</i>
Empirical formula	C <sub>18</sub> H <sub>16</sub> Cl <sub>6</sub> N <sub>2</sub> S <sub>2</sub> Sn	C <sub>18</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub> S <sub>2</sub> Sn	C <sub>18</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub> S <sub>2</sub> Sn	C <sub>19</sub> H <sub>16</sub> Cl <sub>8</sub> N <sub>2</sub> S <sub>2</sub> Sn
Formula weight	655.84	510.01	510.01	738.75
T/K	150(2)	123(2)	123(2)	123(2)
a [Å]	10.2402(11)	15.4999(8)	8.0780(16)	13.870(3)
b [Å]	9.9690(9)	8.4072(4)	9.3260(19)	11.326(2)
c [Å]	12.3557(12)	14.5149(7)	13.252(3)	17.080(3)
α [°]	90	90	96.93(3)	90
β [°]	109.198(12)	107.818(3)	91.63(3)	104.45(3)
γ [°]	90	90	112.90(3)	90
V [Å <sup>3</sup> ]	1191.2(2)	1800.72(16)	909.9(4)	2598.2(10)
Z	2	4	2	4
ρ <sub>cal</sub> /cm <sup>3</sup>	1.829	1.881	1.862	1.889
μ/mm <sup>-1</sup>	1.931	1.951	1.931	1.981
GOF	1.056	1.049	1.039	1.034
2θ range (deg)	5.374 - 49.992	5.896 - 60.518	3.106 - 52.744	4.358 - 63.632
Refs collected	8626	9216	13104	33136
Unique/observed	2091	2683	3693	7332
Parameters	134	114	226	297
<i>R</i> <sub>int</sub>	0.1026	0.0286	0.0891	0.0368
<i>R</i> <sub>I</sub> , w <i>R</i> <sub>2</sub> [ <i>I</i> > 2σ( <i>I</i> )]	0.0552, 0.1068	0.0215, 0.0484	0.0613, 0.1503	0.0312, 0.0789
<i>R</i> <sub>I</sub> , w <i>R</i> <sub>2</sub> [ <i>I</i> > 2σ( <i>I</i> )]	0.0888, 0.1250	0.0254, 0.0503	0.0675, 0.1569	0.0342, 0.0807

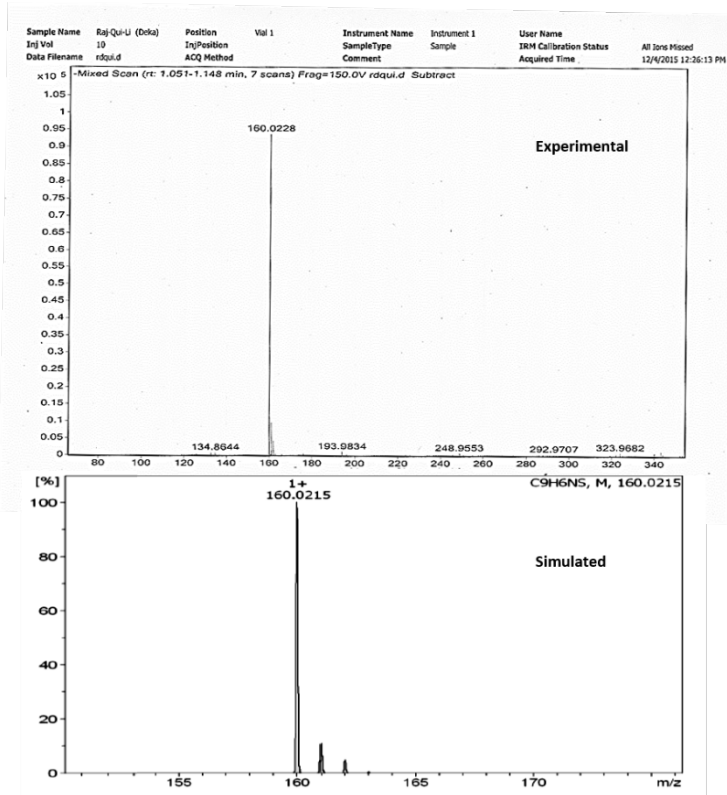
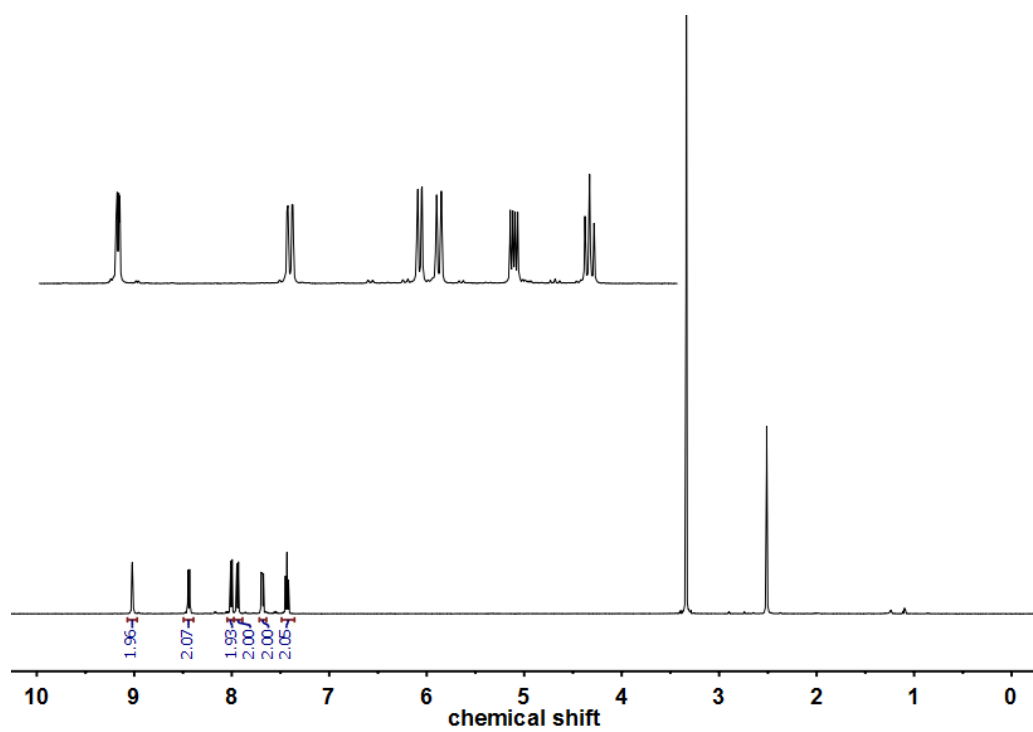
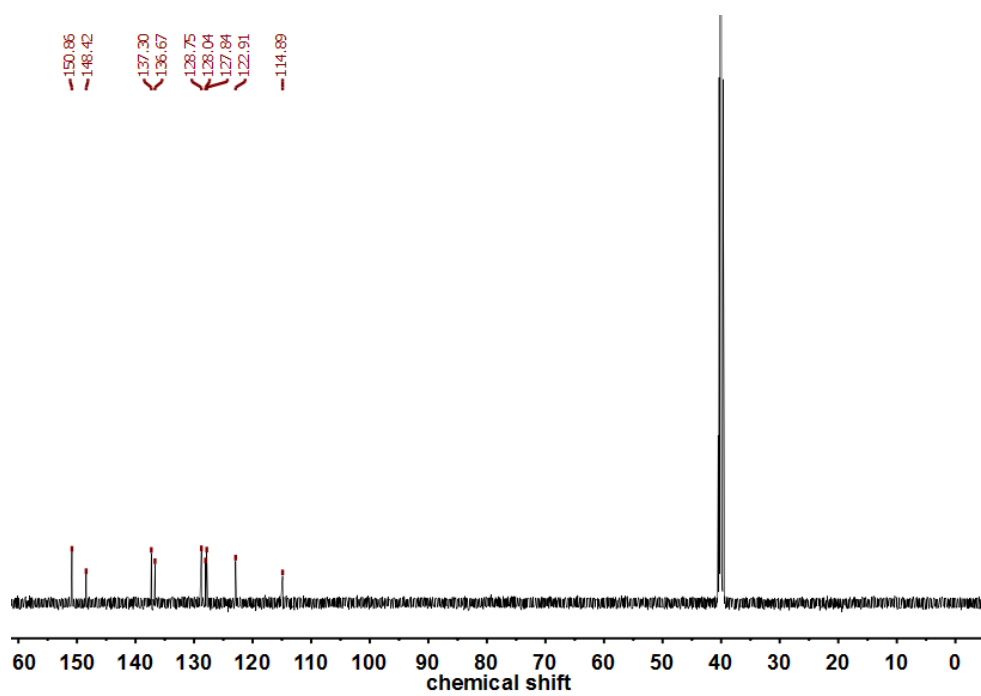


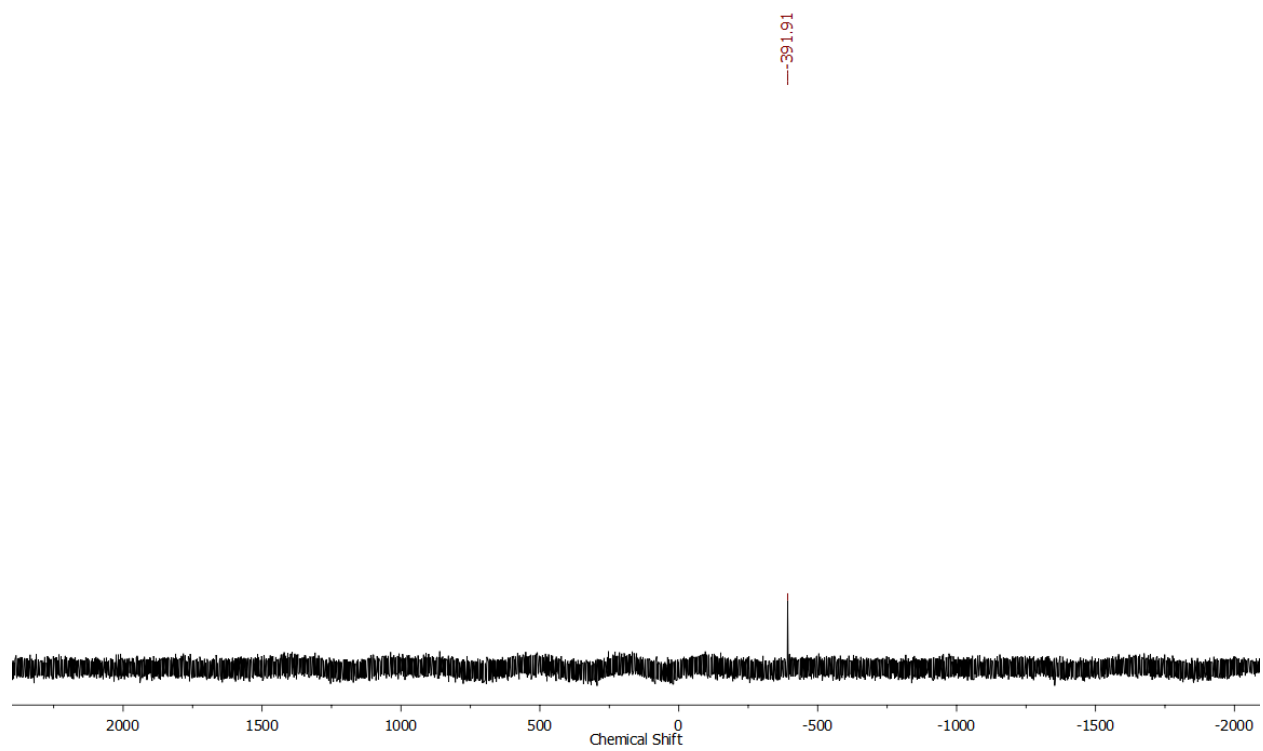
Figure S3. ESI-Mass Spectrum of 2.



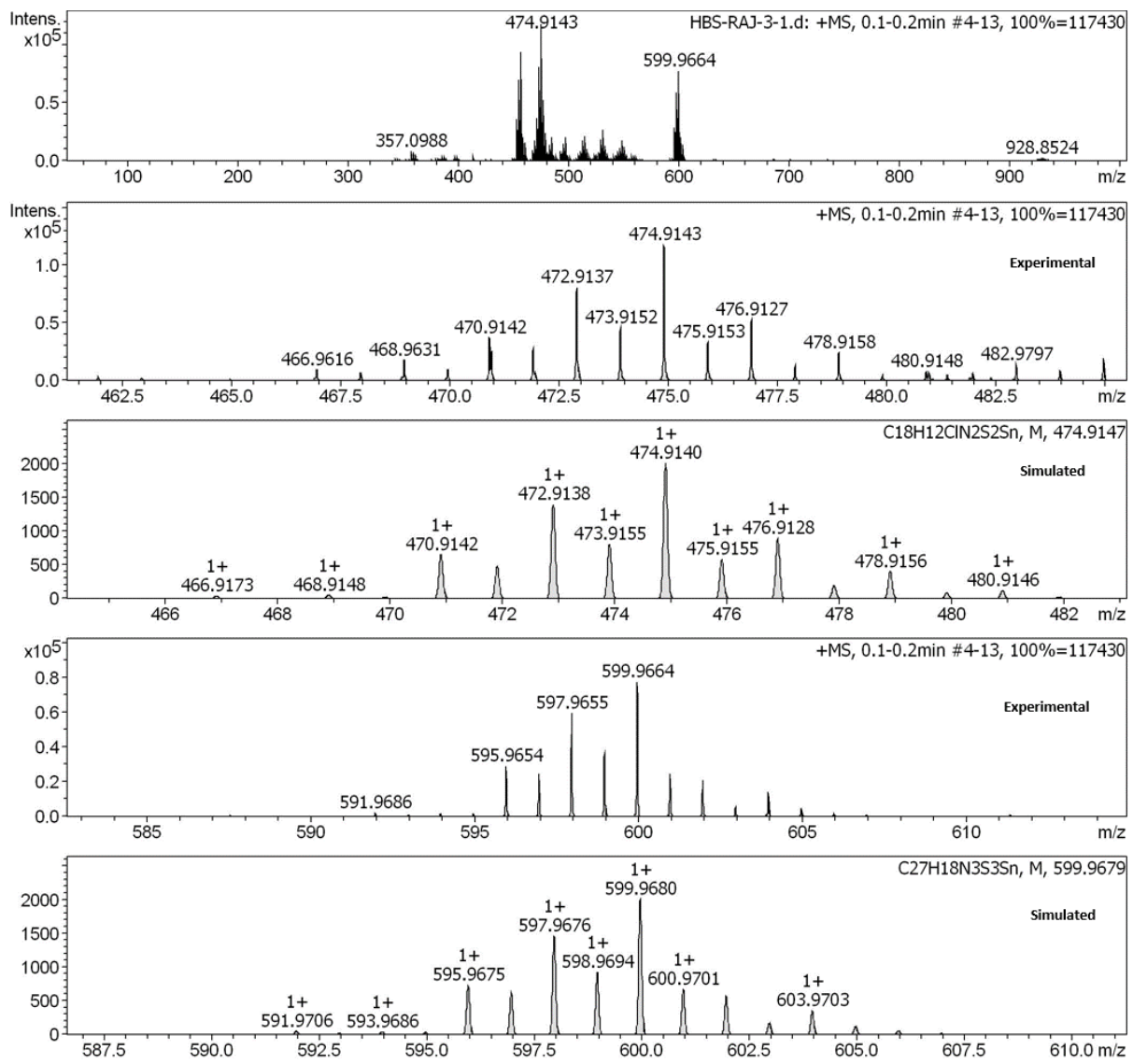
**Figure S4.**  $^1\text{H}$  NMR Spectrum of **3**.



**Figure S5.**  $^{13}\text{C}$  NMR Spectrum of **3**.

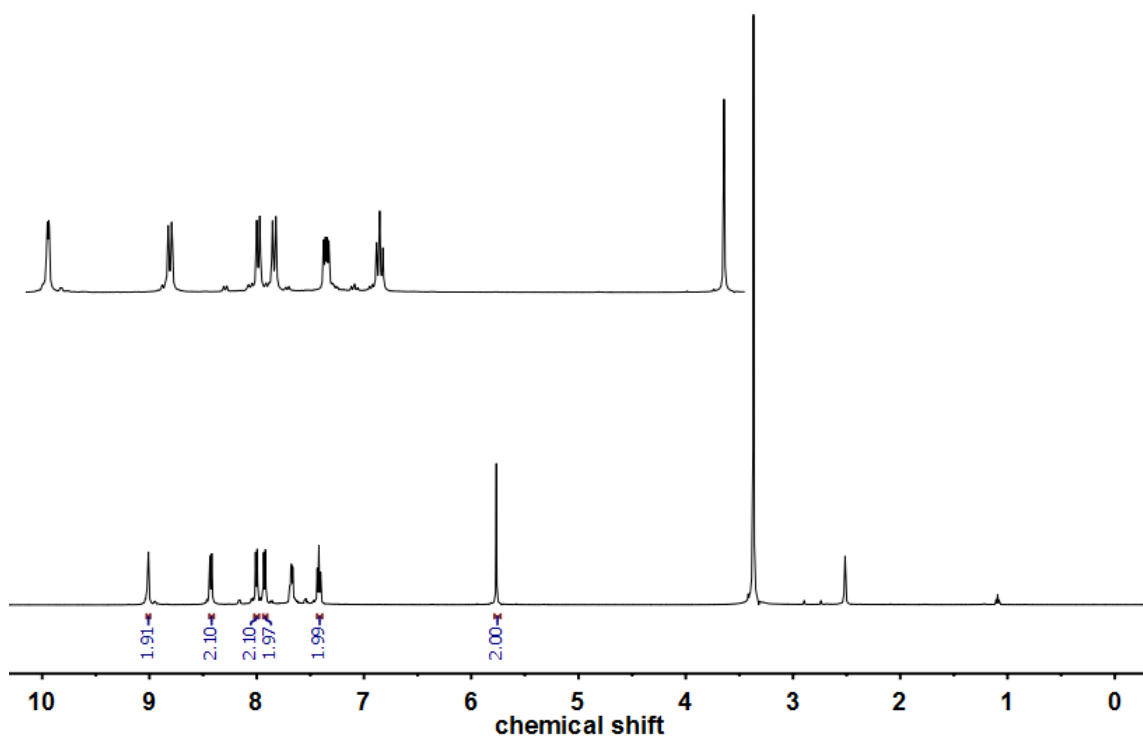


**Figure S6.**  $^{119}\text{Sn}\{^1\text{H}\}$  NMR Spectrum of **3**.



**Figure S7.** ESI-Mass Spectrum of 3.





**Figure S8.** <sup>1</sup>H NMR Spectrum of 4.

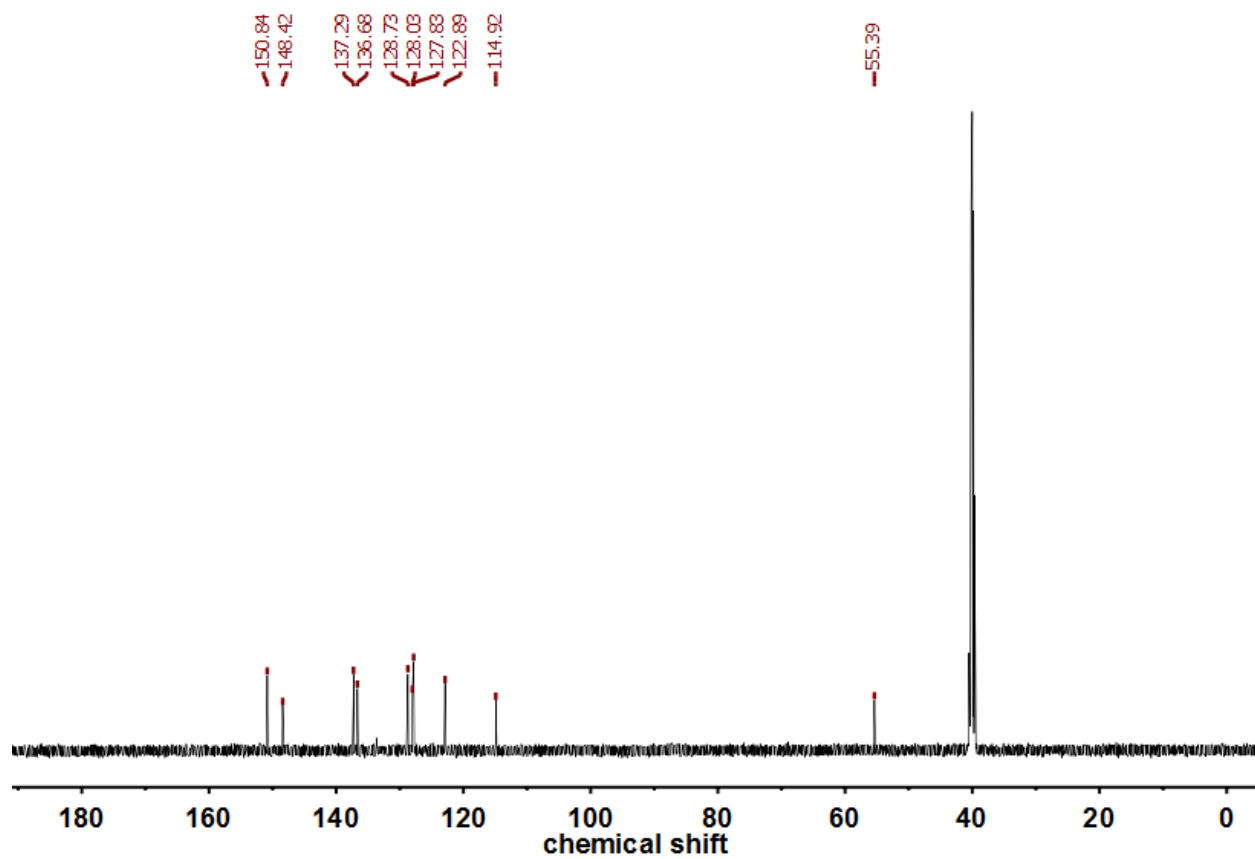


Figure S9.  $^{13}\text{C}$  NMR Spectrum of 4.

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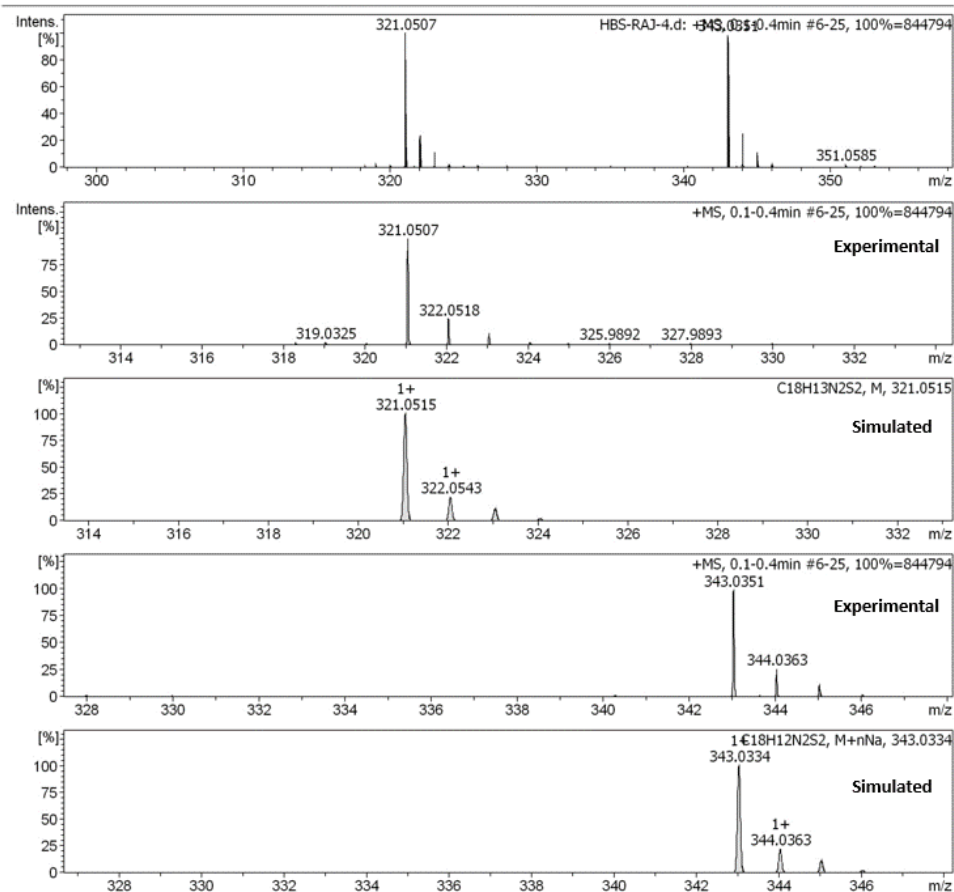
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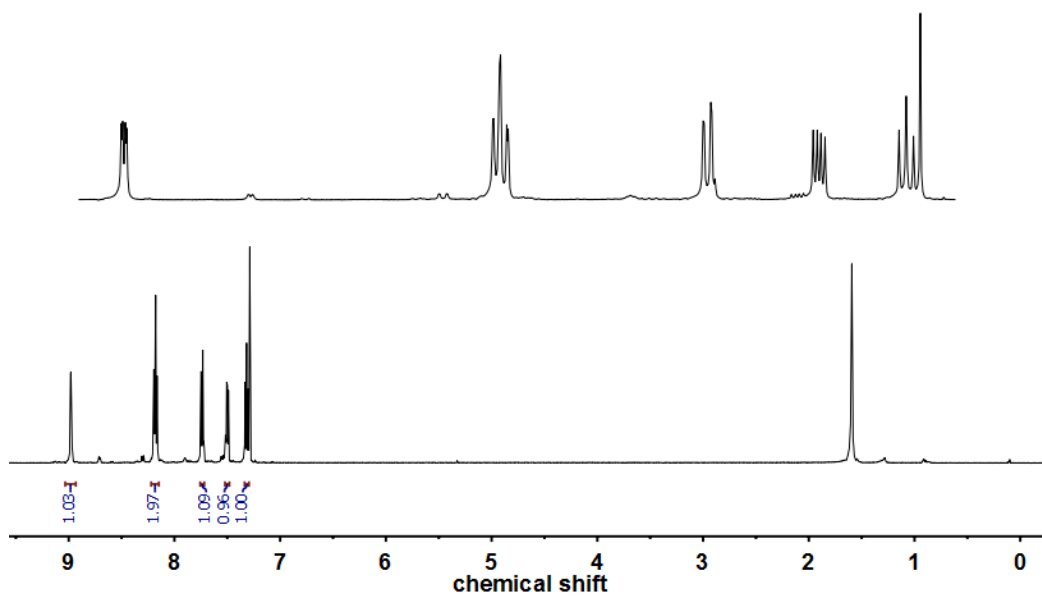
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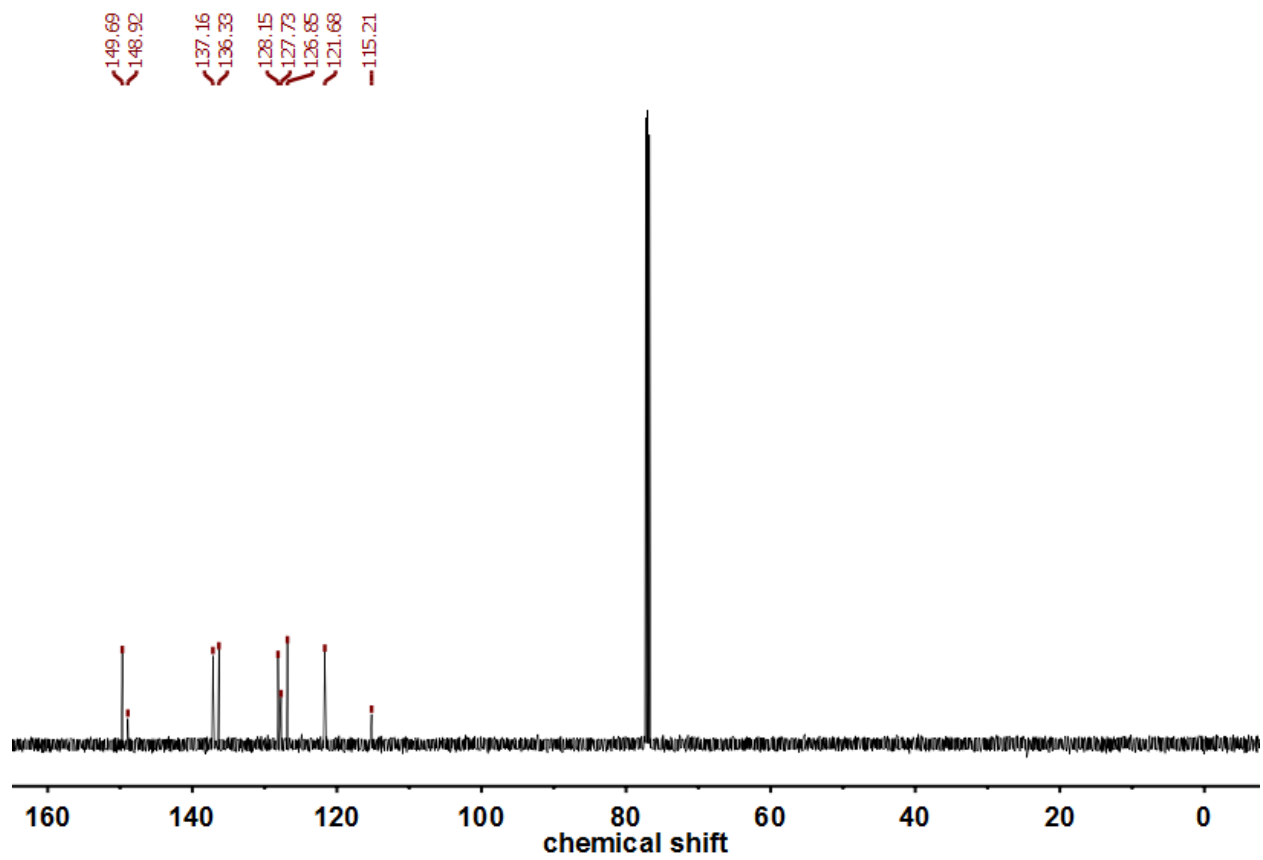
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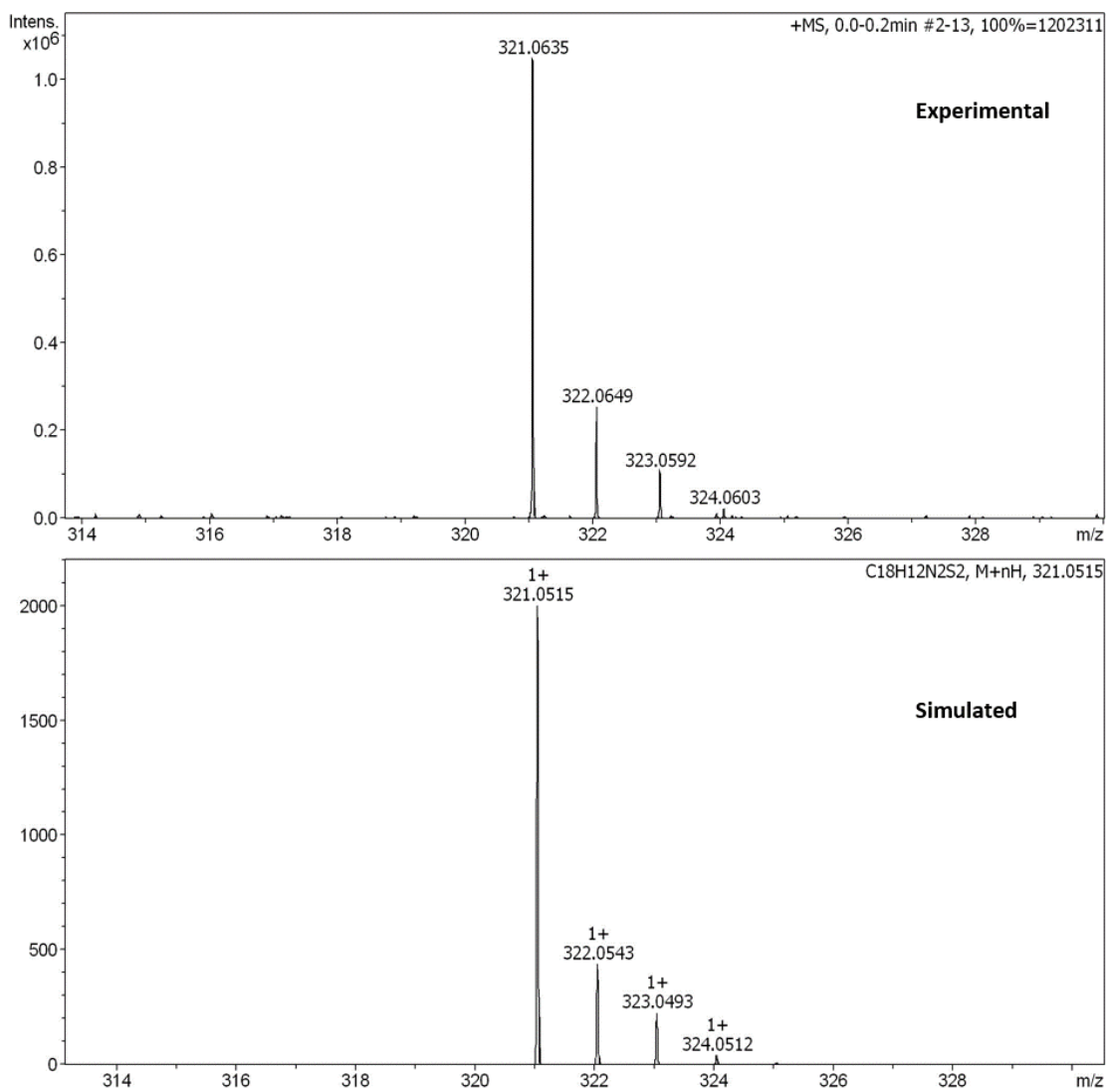
Figure S10. ESI-Mass Spectrum of 4.



**Figure S11.**  $^1\text{H}$  NMR Spectrum of **5**.



**Figure S12.** <sup>13</sup>C NMR Spectrum of 5.



**Figure S13.** ESI-Mass Spectrum of 5.

**Table S2.** Comparison of bond lengths (in Å) and bond angles (in °) between X-ray structures and optimized structures of **2-4**

**Compound 2**

Selected Structural Parameters	X-ray geometry	Optimized geometry
Sn1–Cl3	2.4332	2.529
Sn1–Cl1	2.4121	2.471
Sn1–Cl2	2.4371	2.492
S1–C1	1.772	1.782
Cl1–Sn1–Cl2	90.18	89.63
Cl1–Sn1–Cl3	90.09	89.12
Cl2–Sn1–Cl3	90.57	90.98

**Complex 3m/3t**

Selected Structural Parameters	X-ray geometry		Optimized geometry
	3m	3t	
S1– Sn1	2.4168	2.4401	2.513
S2–Sn1	2.4168	2.4435	2.513
N2– Sn1	2.2876	2.293	2.388
N1– Sn1	2.2875	2.283	2.388
Cl1–Sn1	2.4358	2.4388	2.409
Cl2–Sn1	2.4358	2.4287	2.409
S1–C1	1.7504	1.755	1.761
S2–C18	1.7504	1.765	1.761
N1–Sn1–S1	80.38	80.42	78.13
N2–Sn1–S2	80.38	80.47	78.13
N1–Sn1–Cl1	88.31	90.70	87.66
N2–Sn1–Cl2	88.31	89.96	87.70
N1–Sn1–Cl2	169.12	169.39	162.97
N2–Sn1–Cl1	169.12	167.74	162.94
C1–S1–Sn1	100.25	99.81	100.44
C18–S2–Sn1	100.25	98.92	100.44
Cl1–Sn1–Cl2	91.64	94.48	106.55
N1–Sn1–N2	93.78	86.86	80.07
S1–Sn1–S2	169.35	172.11	165.85

**Compound 4**

<b>Selected Structural Parameters</b>	<b>X-ray geometry</b>	<b>Optimized geometry</b>
Cl1-Sn1	2.4319	2.487
Cl2-Sn1	2.4405	2.602
Cl3-Sn1	2.4640	2.481
Cl4-Sn1	2.4118	2.399
Cl5-Sn1	2.4271	2.397
Cl6-Sn1	2.4208	2.781
S1-S2	2.0554	2.130
S1-C1	1.776	1.785
S2-C10	1.778	1.786
C1-S1-S2	104.85	102.25
C10-S2-S1	103.20	105.15
Cl1-Sn1-Cl2	89.842	86.38
Cl1-Sn1-Cl3	174.52	171.82
Cl1-Sn1-Cl4	91.285	91.45
Cl1-Sn1-Cl5	87.976	93.32
Cl1-Sn1-Cl6	92.78	87.94
Cl2-Sn1-Cl3	88.842	88.58
Cl2-Sn1-Cl4	176.518	164.87
Cl2-Sn1-Cl5	91.41	91.74
Cl2-Sn1-Cl6	86.88	78.56
Cl3-Sn1-Cl4	90.338	91.74
Cl3-Sn1-Cl5	86.74	93.26
Cl3-Sn1-Cl6	92.46	84.75
Cl4-Sn1-Cl5	91.92	103.34
Cl4-Sn1-Cl6	89.77	86.40
Cl5-Sn1-Cl6	178.13	170.12

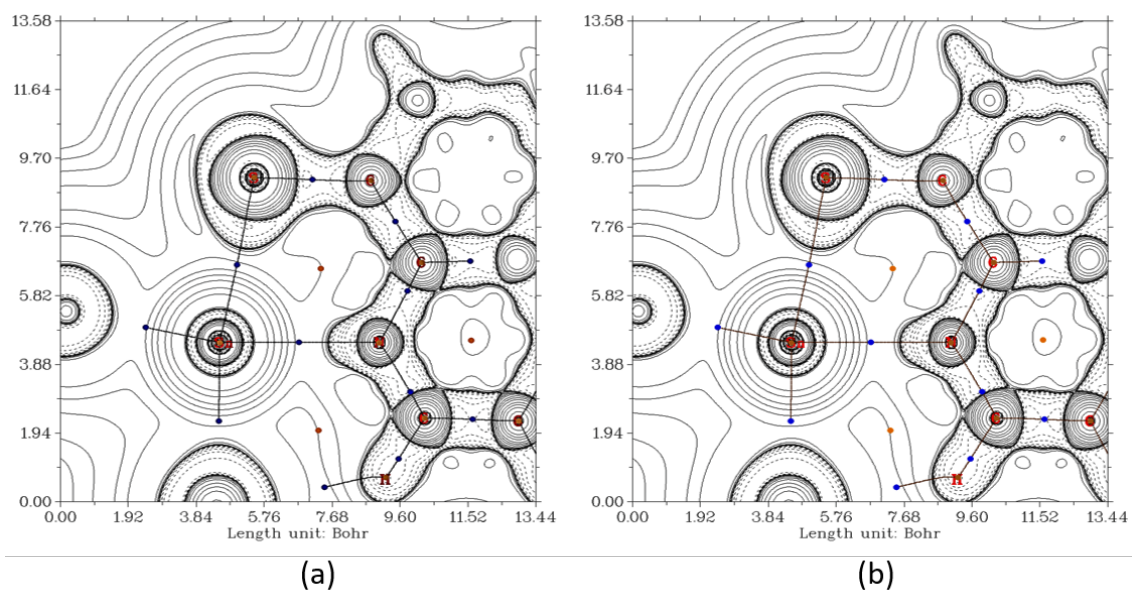


**Table S3:** Donor-Acceptor (Lewis-non-Lewis) type interaction along with their stabilization energy, occupation number (in parenthesis red coloured) and hybridization of complex **3m/3t**

<b>Donor(Lewis) NBO and wave function decomposition</b>	<b>Acceptor (Non-Lewis) NBO and wave function decomposition</b>	<b>Stabilization Energy (kcal/mol)</b>
S1 (LP) – (1.534) – s-16.03% + p-83.79%	Sn1 (LP*) – (1.056)- s-99.71%	419.0
S1 (LP) – (1.534) – s-16.03% + p-83.79%	Sn1 (LP*) – (0.496)- p-100.00%	139.5
S2 (LP) – (1.534) – s-16.03% + p-83.79%	Sn1 (LP*) – (1.056)- s-99.71%	419.0
S2 (LP) – (1.534) – s-16.03% + p-83.79%	Sn1 (LP*) – (0.496)- p-100.00%	139.5
N1 (LP) – (1.790) – s-21.61% + p-78.38%	Sn1 (LP*) – (1.056)- s-99.71%	58.8
N1 (LP) – (1.790) – s-21.61% + p-78.38%	Sn1 (LP*) – (0.415)- p-100.00%	19.3
N1 (LP) – (1.790) – s-21.61% + p-78.38%	Sn1 (LP*) – (0.405)- p-99.85%	33.7
N2 (LP) – (1.790) – s-21.61% + p-78.38%	Sn1 (LP*) – (1.056)- s-99.71%	58.8
N2 (LP) – (1.790) – s-21.61% + p-78.38%	Sn1 (LP*) – (0.415)- p-100.00%	19.3
N2 (LP) – (1.790) – s-21.61% + p-78.38%	Sn1 (LP*) – (0.405)- p-99.85%	33.7
C11 (LP) – (1.603) – s-19.32%+ p-80.49%	Sn1 (LP*) – (1.056)- s-99.71%	136.0
C11 (LP) – (1.603) – s-19.32%+ p-80.49%	Sn1 (LP*) – (0.415)- p-100.00%	88.6
C11 (LP) – (1.603) – s-19.32%+ p-80.49%	Sn1 (LP*) – (0.405)- p-99.85%	43.6
C12 (LP) – (1.603) – s-19.32%+ p-80.49%	Sn1 (LP*) – (1.056)- s-99.71%	136.0
C12 (LP) – (1.603) – s-19.32%+ p-80.49%	Sn1 (LP*) – (0.415)- p-100.00%	88.6
C12 (LP) – (1.603) – s-19.32%+ p-80.49%	Sn1 (LP*) – (0.405)- p-99.85%	43.6

**Table S4.** S-Sn Bond critical points for the **3m** and **3t**.

Compounds	$\rho(r)$	$\nabla^2\rho(r)$	$V(r)$	$G(r)$	$H(r)$
<b>3m</b>	0.06740	0.10041	-0.03068	-0.01371	-0.01697
	0.06740	0.10041	-0.03068	-0.01371	-0.01697
<b>3t</b>	0.06742	0.10045	-0.03690	-0.01371	-0.01698
	0.06742	0.10045	-0.03690	-0.01371	-0.01698



**Figure S14.** Laplacian of electron density [ $\nabla^2\rho(r)$ ] plots for (a) **3m** and (b) **3t**.

### Cartesian Coordinates for 2

Sn	0.000000000	0.000000000	0.000000000
Cl	-1.599893000	-1.641196000	-1.067889000
Cl	0.899284000	-1.837227000	1.386303000
Cl	1.723040000	-0.486077000	-1.733092000
Cl	1.599893000	1.641196000	1.067889000
Cl	-0.899284000	1.837227000	-1.386303000
Cl	-1.723040000	0.486077000	1.733092000
S	0.938775000	-3.807812000	-3.002086000
H	1.140785000	-2.802481000	-2.099078000
N	-0.474534000	-1.174367000	-3.867564000
H	-0.688659000	-1.694641000	-2.986857000
C	0.787148000	-0.820005000	-5.867039000
C	0.511944000	-1.609819000	-4.708755000
C	1.765114000	-1.271308000	-6.791410000
H	1.973973000	-0.669646000	-7.678688000
C	1.246335000	-2.803822000	-4.442309000
C	0.066695000	0.393807000	-6.038199000
H	0.287750000	1.015815000	-6.909682000
C	2.187846000	-3.201610000	-5.382235000
H	2.763309000	-4.109401000	-5.189728000
C	-0.885101000	0.789957000	-5.121880000
H	-1.429653000	1.729061000	-5.218553000
C	-1.145320000	-0.042091000	-4.020829000

H	-1.861234000	0.195049000	-3.232466000
C	2.437925000	-2.451158000	-6.554933000
H	3.192315000	-2.804360000	-7.261506000
S	-0.938775000	3.807812000	3.002086000
H	-1.140785000	2.802481000	2.099078000
N	0.474534000	1.174367000	3.867564000
H	0.688659000	1.694641000	2.986857000
C	-0.787148000	0.820005000	5.867039000
C	-0.511944000	1.609819000	4.708755000
C	-1.765114000	1.271308000	6.791410000
H	-1.973973000	0.669646000	7.678688000
C	-1.246335000	2.803822000	4.442309000
C	-0.066695000	-0.393807000	6.038199000
H	-0.287750000	-1.015815000	6.909682000
C	-2.187846000	3.201610000	5.382235000
H	-2.763309000	4.109401000	5.189728000
C	0.885101000	-0.789957000	5.121880000
H	1.429653000	-1.729061000	5.218553000
C	1.145320000	0.042091000	4.020829000
H	1.861234000	-0.195049000	3.232466000
C	-2.437925000	2.451158000	6.554933000
H	-3.192315000	2.804360000	7.261506000

### Cartesian Coordinates for 3m

Sn	-0.000008000	1.290932000	-0.000010000
Cl	1.233673000	2.732048000	-1.485301000
S	1.777038000	0.981248000	1.750082000
N	1.252122000	-0.537112000	-0.889400000
C	2.784480000	-0.234473000	0.969884000
C	3.988237000	-0.606032000	1.564773000
H	4.287891000	-0.114466000	2.493051000
C	4.824940000	-1.593909000	1.003925000
H	5.758323000	-1.847733000	1.512321000
C	4.478833000	-2.232878000	-0.168912000
H	5.121445000	-2.998805000	-0.608892000
C	3.268142000	-1.886772000	-0.821791000
C	2.412585000	-0.880103000	-0.258675000
C	0.894505000	-1.120521000	-2.021036000
H	-0.041655000	-0.770977000	-2.467393000
C	1.673141000	-2.124922000	-2.632484000
H	1.332046000	-2.576245000	-3.565556000
C	2.855008000	-2.500640000	-2.033057000
H	3.491050000	-3.269537000	-2.480200000
Cl	-1.233648000	2.732126000	1.485227000
S	-1.777061000	0.981224000	-1.750103000
N	-1.252139000	-0.537057000	0.889421000
C	-2.784490000	-0.234494000	-0.969884000

C	-3.988238000	-0.606092000	-1.564769000
H	-4.287896000	-0.114557000	-2.493061000
C	-4.824925000	-1.593971000	-1.003900000
H	-5.758300000	-1.847827000	-1.512293000
C	-4.478810000	-2.232905000	0.168955000
H	-5.121410000	-2.998834000	0.608950000
C	-3.268130000	-1.886758000	0.821834000
C	-2.412593000	-0.880086000	0.258697000
C	-0.894510000	-1.120433000	2.021071000
H	0.041653000	-0.770875000	2.467410000
C	-1.673129000	-2.124832000	2.632540000
H	-1.332027000	-2.576126000	3.565624000
C	-2.854987000	-2.500587000	2.033117000
H	-3.491013000	-3.269487000	2.480276000

**Cartesian Coordinates for 3t**

Sn	0.000075000	1.291043000	-0.000017000
Cl	-1.234201000	2.730951000	1.486044000
Cl	1.233420000	2.732541000	-1.485179000
S	-1.776852000	0.981394000	-1.750013000
S	1.777057000	0.981409000	1.749905000
N	1.252304000	-0.536891000	-0.889598000
N	-1.252069000	-0.537223000	0.889347000
C	2.412674000	-0.879997000	-0.258760000
C	1.673402000	-2.124711000	-2.632658000

H	1.332382000	-2.576008000	-3.565766000
C	0.894765000	-1.120275000	-2.021271000
H	-0.041401000	-0.770789000	-2.467623000
C	-2.412504000	-0.880156000	0.258559000
C	3.268197000	-1.886747000	-0.821767000
C	3.988100000	-0.606123000	1.564938000
H	4.287677000	-0.114624000	2.493267000
C	-2.784293000	-0.234505000	-0.970027000
C	2.855180000	-2.500535000	-2.033111000
H	3.491182000	-3.269494000	-2.480184000
C	2.784490000	-0.234426000	0.969864000
C	-3.268145000	-1.886796000	0.821580000
C	4.824769000	-1.594095000	1.004186000
H	5.758032000	-1.848063000	1.512719000
C	4.478759000	-2.233001000	-0.168711000
H	5.121356000	-2.998978000	-0.608607000
C	-3.987966000	-0.606023000	-1.565076000
H	-4.287535000	-0.114434000	-2.493358000
C	-2.855196000	-2.500606000	2.032942000
H	-3.491293000	-3.269471000	2.480039000
C	-4.478764000	-2.232888000	0.168549000
H	-5.121454000	-2.998782000	0.608455000
C	-0.894596000	-1.120603000	2.021026000
H	0.041604000	-0.771222000	2.467389000
C	-4.824731000	-1.593921000	-1.004327000

H	-5.758049000	-1.847756000	-1.512829000
C	-1.673383000	-2.124892000	2.632483000
H	-1.332444000	-2.576161000	3.565636000

#### **Cartesian Coordinates for 4**

Sn	3.144661000	0.054987000	0.095786000
Cl	3.099069000	-2.416065000	0.377384000
Cl	1.303918000	-0.282492000	-1.712002000
Cl	2.839536000	2.506290000	-0.139437000
Cl	4.347062000	0.328219000	2.153224000
Cl	4.881796000	-0.025105000	-1.553610000
Cl	0.831539000	0.172472000	1.635492000
S	-2.514340000	0.641816000	2.300563000
S	-3.685319000	-1.137314000	2.282747000
N	-1.074136000	1.893872000	-0.094137000
H	-0.566460000	1.306625000	0.634325000
N	-1.187790000	-1.988319000	0.436438000
H	-1.020472000	-1.393789000	1.263782000
C	-0.284899000	2.372365000	-1.048785000
H	0.788274000	2.183379000	-0.938504000
C	-0.819396000	3.133824000	-2.107228000
H	-0.139792000	3.512438000	-2.871242000
C	-2.172244000	3.374085000	-2.138584000
H	-2.617047000	3.960467000	-2.947072000
C	-3.022236000	2.870920000	-1.111427000



C	-2.433797000	2.104226000	-0.056706000
C	-3.259999000	1.599504000	0.989955000
C	-4.624531000	1.860242000	0.957680000
H	-5.250156000	1.467066000	1.761812000
C	-5.208333000	2.600681000	-0.089569000
H	-6.284828000	2.784136000	-0.082631000
C	-4.420790000	3.102356000	-1.107031000
H	-4.859818000	3.685553000	-1.919617000
C	-0.082389000	-2.423335000	-0.158943000
H	0.872047000	-2.231072000	0.341793000
C	-0.150227000	-3.140047000	-1.369390000
H	0.789631000	-3.476220000	-1.806919000
C	-1.374875000	-3.315101000	-1.961789000
H	-1.463755000	-3.830559000	-2.921467000
C	-2.561247000	-2.815196000	-1.341743000
C	-2.452198000	-2.157252000	-0.080004000
C	-3.627284000	-1.717280000	0.595466000
C	-4.858425000	-1.871770000	-0.038681000
H	-5.755852000	-1.515412000	0.470925000
C	-4.969567000	-2.496727000	-1.297622000
H	-5.953450000	-2.608500000	-1.757704000
C	-3.840935000	-2.972449000	-1.932873000
H	-3.912776000	-3.475101000	-2.900046000