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Supplementary Information

A Serendipitous Isolation of Cocrystalized Platinum-Tin Complexes: Synthesis, Structure and Theoretical Exploration

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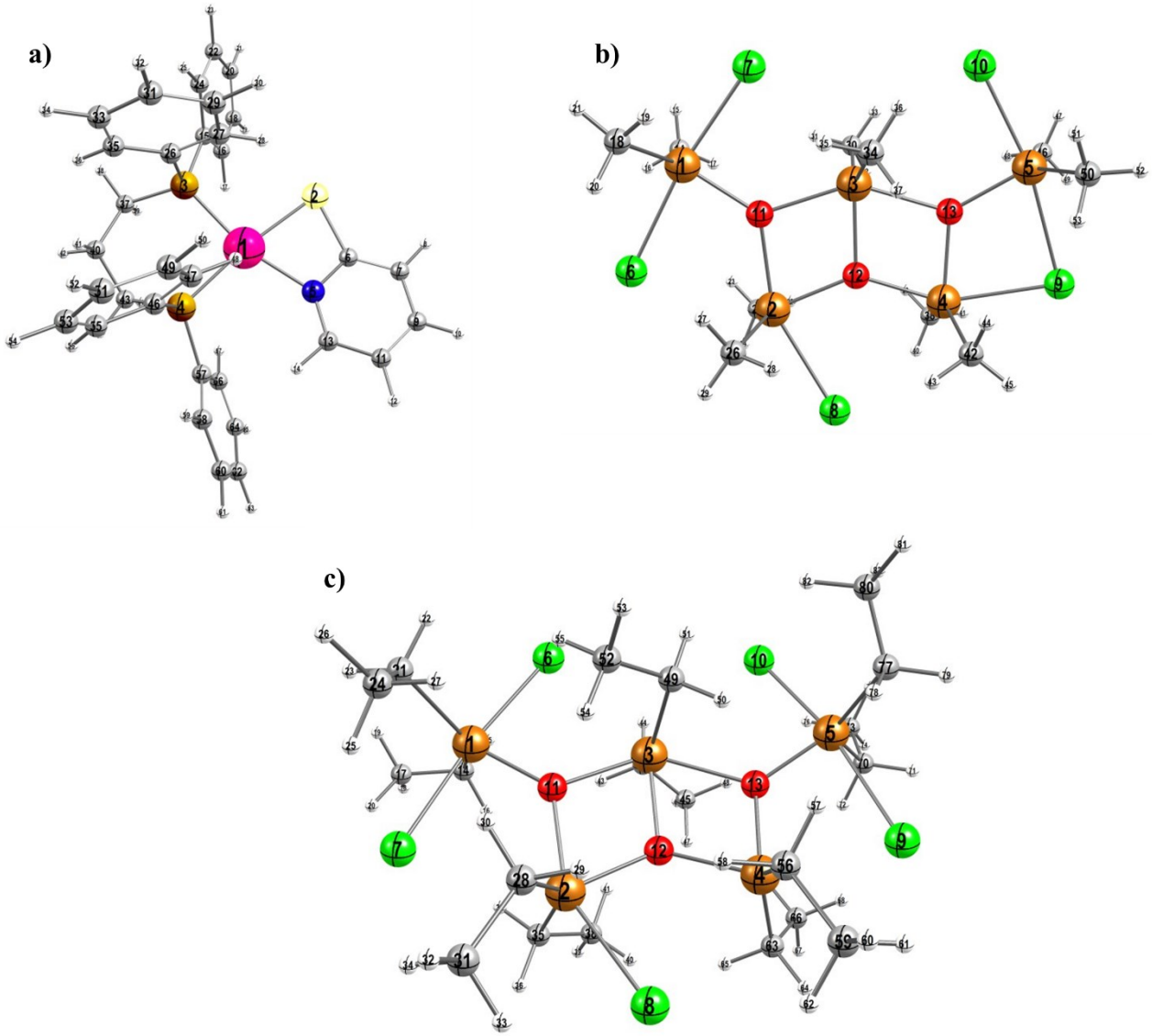

Figure S1. DFT optimized geometries a) [{Pt(κ$_2$-SeC$_5$H$_4$N)(dppp)}]; b) [{(Me$_2$Sn)$_5$O$_3$Cl$_5$}] ;c) [{(Me$_2$Sn)$_5$O$_3$Cl$_5$}]. The labelling of atoms are for comparing NPA charges and second order perturbation analysis donor-acceptor interaction analysis. Color code: Pt (pink), Sn (tangerine), P(light brown), Se (light yellow), Cl (green), O (red), N(blue), C (grey) and H (white).

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Table S1. NBO computed NPA charges on crystal structure and DFT optimized geometry of **[{Pt(κ_2-SeC_5H_4N)(dppp)}]** unit of complex **2a**. Pt and atoms in first coordination sphere were kept in bold. (For numbering see Figure S1)

Atoms	**[{Pt(κ_2-SeC_5H_4N)(dppp)}]** *(X-ray Crystal Structure)*	**[{Pt(κ_2-SeC_5H_4N)(dppp)}]** *(DFT Optimized Geometry)*
Pt 1	**0.13772**	**0.14654**
Se 2	**-0.06074**	**-0.05301**
P 3	**1.10344**	**1.09997**
P 4	**1.02434**	**1.03107**
N 5	**-0.55618**	**-0.57108**
C 6	0.07807	0.07738
C 7	-0.23095	-0.27305
H 8	0.21661	0.26914
C 9	-0.09103	-0.16336
H 10	0.20361	0.26198
C 11	-0.23445	-0.28436
H 12	0.20663	0.26224
C 13	0.14653	0.08273
H 14	0.18636	0.24367
C 15	-0.36143	-0.36941
C 16	-0.18422	-0.22953
H 17	0.20419	0.25609
C 18	-0.15634	-0.21946
H 19	0.19962	0.25507
C 20	-0.15209	-0.20777
H 21	0.19739	0.25470
C 22	-0.16892	-0.21991
H 23	0.20041	0.25442
C 24	-0.15973	-0.21700
H 25	0.19758	0.25541
C 26	-0.36986	-0.37056
C 27	-0.16269	-0.21995
H 28	0.20324	0.26372
C 29	-0.16504	-0.22762
H 30	0.20048	0.25531
C 31	-0.14855	-0.21227
H 32	0.19756	0.25403
C 33	-0.17425	-0.21971
H 34	0.20020	0.25404
C 35	-0.17679	-0.22022
H 36	0.19196	0.24175
C 37	-0.69499	-0.75848
H 38	0.24546	0.28473
H 39	0.24714	0.28296
C 40	-0.38058	-0.47744
H 41	0.21276	0.25149
H 42	0.22988	0.27222
C 43	-0.67133	-0.74775
H 44	0.23638	0.27804
H 45	0.24075	0.27901
C 46	-0.37763	-0.37946
C 47	-0.15417	-0.21050
H 48	0.20113	0.25723
C 49	-0.16305	-0.22216
H 50	0.19942	0.25503
C 51	-0.15755	-0.20633
H 52	0.19829	0.25417

C 53	-0.16248	-0.22494
H 54	0.20108	0.25510
C 55	-0.17921	-0.22945
H 56	0.19685	0.24654
C 57	-0.37910	-0.37284
C 58	-0.17235	-0.22668
H 59	0.20059	0.25967
C 60	-0.16371	-0.22282
H 61	0.20032	0.25658
C 62	-0.16555	-0.21388
H 63	0.20095	0.25657
C 64	-0.16341	-0.22074
H 65	0.20313	0.25681
C 66	-0.16855	-0.22575
H 67	0.19685	0.25206

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Table S2. NBO computed NPA charges on DFT optimized geometry of [{Pt(κ_2-SeC_5H_4N)(dppp)}] unit of complex **2a** and their isolated fragments {Pt(dppp)} and {SeC_5H_4N}. Pt and atoms in first coordination sphere were kept in bold.

[{Pt(κ_2-SeC_5H_4N)(dppp)}]$^+$		{Pt(dppp)}$^{2+}$		{SeC_5H_4N}	
Pt 1	**0.14654**	**Pt 1**	**0.13767**	**Se 1**	**-0.51484**
Se 2	**-0.05301**	**P 2**	**1.21965**	**N 2**	**-0.51253**
P 3	**1.09997**	**P 3**	**1.21039**	C 3	0.04373
P 4	**1.03107**	C 4	-0.38763	C 4	-0.30171
N 5	**-0.57108**	C 5	-0.22044	H 5	0.23272
C 6	0.07738	H 6	0.24782	C 6	-0.23091
C 7	-0.27305	C 7	-0.20830	H 7	0.21427
H 8	0.26914	H 8	0.27281	C 8	-0.35558
C 9	-0.16336	C 9	-0.16501	H 9	0.20794
H 10	0.26198	H 10	0.27488	C 10	0.02201
C 11	-0.28436	C 11	-0.20125	H 11	0.19489
H 12	0.26224	H 12	0.27473		
C 13	0.08273	C 13	-0.20482		
H 14	0.24367	H 14	0.26522		
C 15	-0.36941	C 15	-0.39364		
C 16	-0.22953	C 16	-0.21857		
H 17	0.25609	H 17	0.25249		
C 18	-0.21946	C 18	-0.21637		
H 19	0.25507	H 19	0.27192		
C 20	-0.20777	C 20	-0.18116		
H 21	0.25470	H 21	0.27229		
C 22	-0.21991	C 22	-0.20690		
H 23	0.25442	H 23	0.27119		
C 24	-0.21700	C 24	-0.21059		
H 25	0.25541	H 25	0.24881		
C 26	-0.37056	C 26	-0.75895		
C 27	-0.21995	H 27	0.31459		
H 28	0.26372	H 28	0.29601		
C 29	-0.22762	C 29	-0.48419		
H 30	0.25531	H 30	0.25987		
C 31	-0.21227	H 31	0.29568		
H 32	0.25403	C 32	-0.75212		
C 33	-0.21971	H 33	0.28994		
H 34	0.25404	H 34	0.30952		
C 35	-0.22022	C 35	-0.40244		
H 36	0.24175	C 36	-0.21071		
C 37	-0.75848	H 37	0.24761		
H 38	0.28473	C 38	-0.21617		
H 39	0.28296	H 39	0.26707		
C 40	-0.47744	C 40	-0.18248		
H 41	0.25149	H 41	0.27078		
H 42	0.27222	C 42	-0.21001		
C 43	-0.74775	H 43	0.27319		
H 44	0.27804	C 44	-0.22529		
H 45	0.27901	H 45	0.25487		
C 46	-0.37946	C 46	-0.38546		
C 47	-0.21050	C 47	-0.20136		
H 48	0.25723	H 48	0.26556		
C 49	-0.22216	C 49	-0.20213		
H 50	0.25503	H 50	0.27449		
C 51	-0.20633	C 51	-0.16173		
H 52	0.25417	H 52	0.27481		
C 53	-0.22494	C 53	-0.20910		

H 54 0.25510 C 55 -0.22945 H 56 0.24654 C 57 -0.37284 C 58 -0.22668 H 59 0.25967 C 60 -0.22282 H 61 0.25658 C 62 -0.21388 H 63 0.25657 C 64 -0.22074 H 65 0.25681 C 66 -0.22575 H 67 0.25206	H 54 0.27288 C 55 -0.21791 H 56 0.24800	

Table S3. Second order perturbation calculated strength of donor acceptor interaction (n→σ*) in [{Pt(κ_2-SeC_5H_4N)(dppp)}] unit of complex **2a** along with details of corresponding lone pair and antibonding orbital with its occupancy.

Fragments	*Lp*	M-L* type	Occupancy (M-L *)	$\Delta E_{M\text{-}L^*}$ (kcal/mole)
{Pt(dppp)}/{SeC_5H_4N}	n_{Se}	σ*(Pt-P)	0.556	147.1
	n_N	σ*(Pt-P)	0.382	89.8

Table S4. EDA analysis of [{Pt(κ_2-SeC_5H_4N)(dppp)}] fragment of complex **2a** along with decomposed orbital interaction energies (E_{Orb}) for both crystal structure and DFT optimized geometry.

Fragments	E_{int} (kcal/mole)	E_{orb} (kcal/mole)	E_{steric} (kcal/mole)
{Pt (dppp)}/{(κ_2-SeC_5H_4N)} (X-ray crystal Structure)	-283.2	-164.7	-114.4
		Decomposed ***E_{orb}*** *interactions*	
		-81.3	
		-37.0	
		-9.2	
		-8.0	
{Pt (dppp)}/{(κ_2-SeC_5H_4N)} (DFT optimized structure)	-277.3	-164.3	-113.0
		Decomposed ***E_{orb}*** *interactions*	
		-77.5	
		-37.8	
		-8.2	
		-8.0	

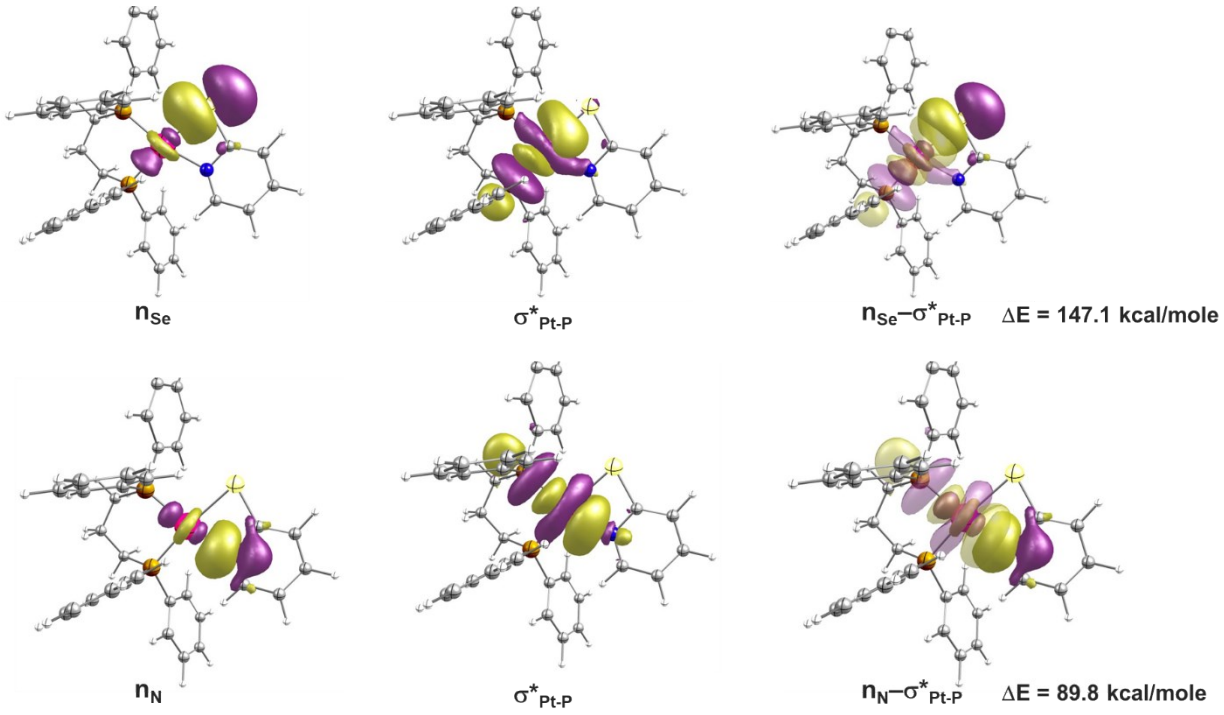

Figure S2. Second order perturbation theory computed two most stabilizing interactions present in [{Pt(κ_2-SeC_5H_4N)(dppp)}] unit of complex **2a**; Three-dimensional contour plots for 3c-4e bonding in (P-Pt…Se) which includes the lone pair of Se i.e. 1c/1e donor (left), formal σ*Pt-P orbital (middle) and the overlap between the lone pair and σ*Pt-P orbital is plotted on the right side; the figure below is for 3c-4e bonding in (P-Pt…N) interaction.

Table S5. NBO computed NPA charges on crystal structure and DFT optimized geometry of **[{(Me$_2$Sn)$_5$O$_3$Cl$_5$}]** unit of complex **2a**. (For numbering see Figure S1)

Atoms	**[{(Me$_2$Sn)$_5$O$_3$Cl$_5$}]** *(X-ray Crystal Structure)*	**[{(Me$_2$Sn)$_5$O$_3$Cl$_5$}]** *(DFT Optimized Geometry)*
Sn	1.74902	1.79094
Sn	1.90083	1.91683
Sn	1.96910	2.02771
Sn	1.90001	1.97672
Sn	1.74532	1.79731
Cl	-0.66189	-0.64378
Cl	-0.64394	-0.62379
Cl	-0.71654	-0.65420
Cl	-0.62504	-0.63232
Cl	-0.59738	-0.59245
O	-1.20264	-1.19467
O	-1.21424	-1.21185
O	-1.19626	-1.18400
C	-1.02428	-1.15811
H	0.22659	0.26378
H	0.22835	0.25958
H	0.22781	0.25877
C	-1.03262	-1.15473
H	0.23387	0.26108
H	0.23223	0.26108
H	0.22525	0.26062
C	-1.03432	-1.16623
H	0.22900	0.27309
H	0.23380	0.26436
H	0.22202	0.25143
C	-1.04145	-1.15840
H	0.22739	0.27240
H	0.22688	0.25677
H	0.23572	0.26241
C	-1.04662	-1.17925
H	0.23182	0.25986
H	0.22030	0.24513
H	0.24212	0.27573
C	-1.04535	-1.17472
H	0.23289	0.26263
H	0.24015	0.27690
H	0.21815	0.25327
C	-1.03411	-1.17121
H	0.22798	0.25617
H	0.24475	0.26340
H	0.22983	0.26752
C	-1.03460	-1.17071
H	0.24302	0.27344
H	0.22133	0.25756
H	0.23162	0.26407
C	-1.02550	-1.15906
H	0.22976	0.26052
H	0.23701	0.26098
H	0.23426	0.26511
C	-1.01294	-1.15516
H	0.23386	0.26168
H	0.22515	0.26175
H	0.23252	0.26406

Table S6. NBO computed NPA charges on crystal structure and DFT optimized geometry of **[{(Et$_2$Sn)$_5$O$_3$Cl$_5$}]** unit of complex **2b**. (For numbering see Figure S1)

Atoms	**[{(Et$_2$Sn)$_5$O$_3$Cl$_5$}]** *(X-ray Crystal Structure)*	**[{(Et$_2$Sn)$_5$O$_3$Cl$_5$}]** *(DFT Optimized Geometry)*
Sn 1	1.78508	1.84192
Sn 2	1.95514	2.00537
Sn 3	2.05219	2.13025
Sn 4	1.93530	2.06758
Sn 5	1.78084	1.83468
Cl 6	-0.63949	-0.62018
Cl 7	-0.64465	-0.64390
Cl 8	-0.70959	-0.65812
Cl 9	-0.64507	-0.63300
Cl 10	-0.54498	-0.58640
O 11	-1.22557	-1.24044
O 12	-1.24093	-1.27413
O 13	-1.20806	-1.23150
C 14	-0.81986	-0.91465
H 15	0.22298	0.26278
H 16	0.21947	0.25247
C 17	-0.59381	-0.69602
H 18	0.19628	0.22540
H 19	0.19316	0.22411
H 20	0.21484	0.25002
C 21	-0.82409	-0.90913
H 22	0.22584	0.26354
H 23	0.21993	0.25075
C 24	-0.59078	-0.69559
H 25	0.20777	0.25293
H 26	0.19240	0.22456
H 27	0.20521	0.22970
C 28	-0.83599	-0.91690
H 29	0.21305	0.24783
H 30	0.22318	0.25682
C 31	-0.59116	-0.69773
H 32	0.19180	0.22406
H 33	0.21564	0.24599
H 34	0.20454	0.24139
C 35	-0.82721	-0.92566
H 36	0.22553	0.25880
H 37	0.21710	0.26376
C 38	-0.59235	-0.68590
H 39	0.19715	0.22669
H 40	0.21215	0.23741
H 41	0.19184	0.22807
C 42	-0.84398	-0.94948
H 43	0.22386	0.25098
H 44	0.23401	0.27725
C 45	-0.59340	-0.68449
H 46	0.20042	0.22761
H 47	0.20083	0.22606
H 48	0.19517	0.23880
C 49	-0.84724	-0.94619
H 50	0.21028	0.24383
H 51	0.23438	0.27013
C 52	-0.58762	-0.69112
H 53	0.19873	0.22702

H 54	0.19627	0.22810
H 55	0.20234	0.24413
C 56	-0.81379	-0.93305
H 57	0.21378	0.24953
H 58	0.23652	0.25248
C 59	-0.59406	-0.69652
H 60	0.19444	0.22567
H 61	0.20245	0.23958
H 62	0.20288	0.24662
C 63	-0.83362	-0.93841
H 64	0.22792	0.26019
H 65	0.23529	0.26406
C 66	-0.59512	-0.69590
H 67	0.19876	0.22730
H 68	0.20810	0.24682
H 69	0.19559	0.23062
C 70	-0.81443	-0.91044
H 71	0.22340	0.25969
H 72	0.23439	0.26031
C 73	-0.59044	-0.69462
H 74	0.19972	0.22462
H 75	0.20156	0.23218
H 76	0.20971	0.24937
C 77	-0.79974	-0.90961
H 78	0.23054	0.25745
H 79	0.22375	0.25796
C 80	-0.59670	-0.69284
H 81	0.19855	0.22470
H 82	0.20806	0.24621
H 83	0.20364	0.23575

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Table S7. NBO computed NPA charges on DFT optimized geometry of $[Sn(CH_3)_2Cl_2]$ complex and monomer model extracted from $[\{(Me_2Sn)_5O_3Cl_5\}]$ (see Sn@1 centre in Figure S1) unit of complex **2a**.

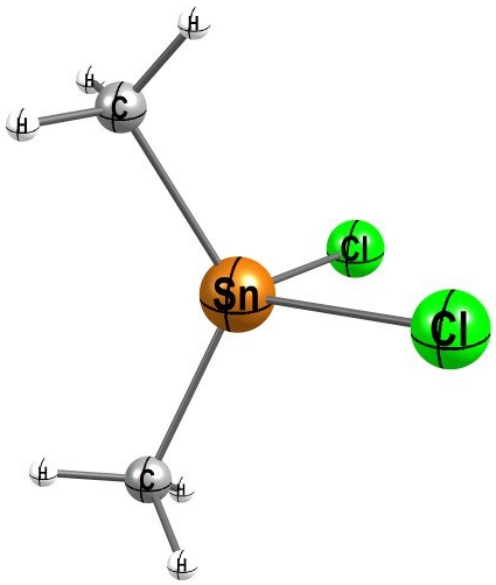
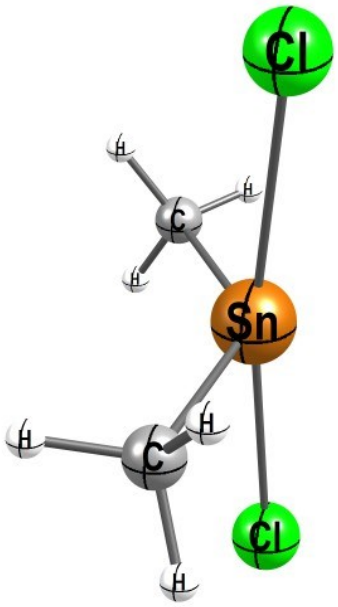
$[Sn(CH_3)_2Cl_2]$ X-ray structure	$[Sn(CH_3)_2Cl_2]$ X-ray structure Sn@1 center in $[\{(Me_2Sn)_5O_3Cl_5\}]$ unit
	
NPA CHARGES Sn 1 1.57567 Cl 2 -0.47170 Cl 3 -0.47136 C 4 -1.13078 H 5 0.26835 H 6 0.27740 H 7 0.26872 C 8 -1.13087 H 9 0.26841 H 10 0.26867 H 11 0.27749	NPA CHARGES Sn 1 1.64401 Cl 2 -0.55099 Cl 3 -0.54040 C 4 -0.99255 H 5 0.24061 H 6 0.24156 H 7 0.23941 C 8 -1.01046 H 9 0.24322 H 10 0.24258 H 11 0.24302

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Table S8. Second order perturbation theory calculated strength of donor acceptor interaction (n→σ*) in [{$(Me_2Sn)_5O_3Cl_5$}] unit of complex **2a** along with the details of corresponding lone pair and antibonding orbital with its occupancy.

Molecule	*Donor*	Acceptor M-L* type	Occupancy (M-L*)	ΔE_{M-L^*} (kcal/mole)
[{$(Me_2Sn)_5O_3Cl_5$}]	n_{Cl} (LP)	σ*(Sn-Cl)	0.182	40.2
	n_{O} (LP)	σ*(Sn-Cl)	0.154	32.5
	n_{O} (LP)	σ*(Sn-O)	0.127	22.8
	n_{O} (LP)	σ*(Sn-O)	0.153	19.41
	n_{O} (LP)	σ*(Sn-O)	0.152	19.07
	n_{Cl} (LP)	σ*(Sn-Cl)	0.144	19.42

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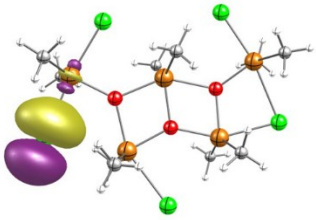
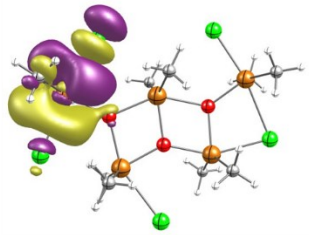
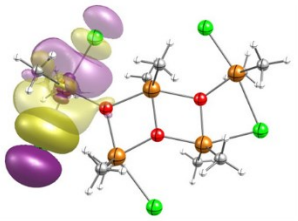


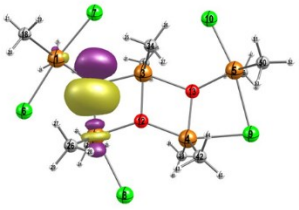
n_{Cl}



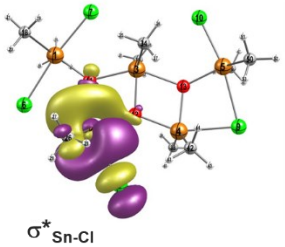
$\sigma^*_{Sn\text{-}Cl}$



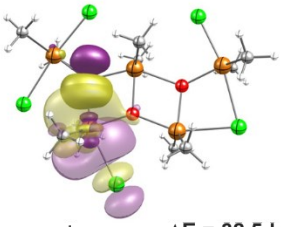
n_{Cl}–$\sigma^*_{Sn\text{-}Cl}$ ΔE = 42.8 kcal/mole



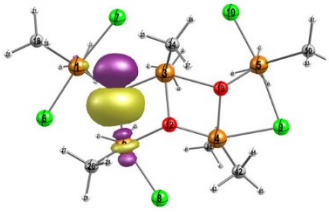
n_O



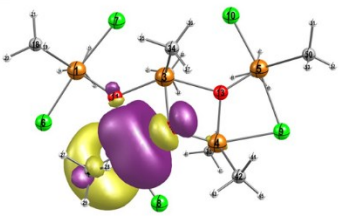
$\sigma^*_{Sn\text{-}Cl}$



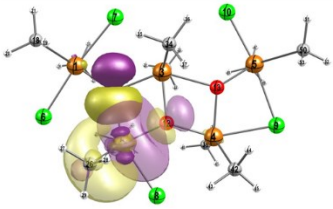
n_O–$\sigma^*_{Sn\text{-}Cl}$ ΔE = 32.5 kcal/mole



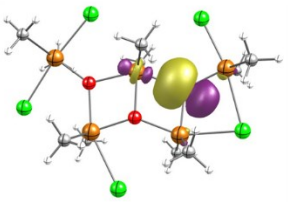
n_O



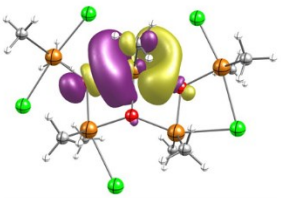
$\sigma^*_{Sn\text{-}O}$



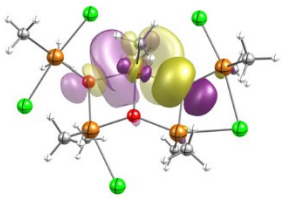
n_O–$\sigma^*_{Sn\text{-}O}$ ΔE = 22.8 kcal/mole



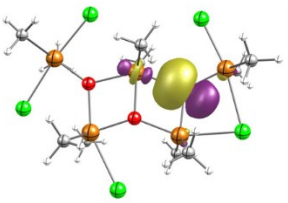
n_O



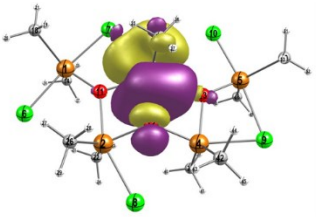
$\sigma^*_{Sn\text{-}O}$



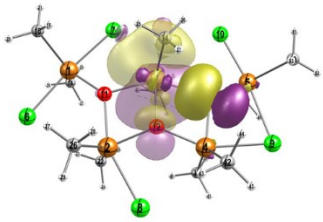
n_O–$\sigma^*_{Sn\text{-}O}$ ΔE =19.4 kcal/mole



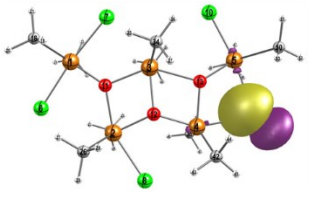
n_O



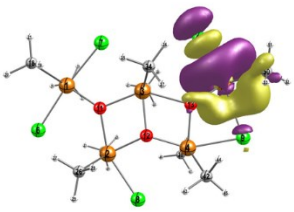
$\sigma^*_{Sn\text{-}O}$



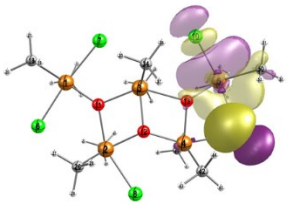
n_O–$\sigma^*_{Sn\text{-}O}$ ΔE = 19.1 kcal/mole



n_{Cl}



$\sigma^*_{Sn\text{-}O}$



n_{Cl}–$\sigma^*_{Sn\text{-}O}$ ΔE = 19.4 kcal/mole

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Figure S3. Second order perturbation theory computed six most stabilizing interactions present in $\{(Me_2Sn)_5O_3Cl_5\}$ core of complex **2a**.These three dimensional contour plots are arranged according to the interactions present in Table S8.

Table S9. EDA analysis of $\{(Me_2Sn)_5O_3Cl_5\}$ fragment of complex **2a** along with decomposed orbital interaction energy (E_{Orb}) for all the three fragments.

Fragments	E_{int} (kcal/mole)	E_{orb} (kcal/mole)	E_{steric} (kcal/mole)
$\{(Me_2Sn)_4O_5Cl_3\}\ldots\{Sn@Cl_2Me_2\}$	-102.5	-105.8	3.34
	Decomposed $\boldsymbol{E_{orb}}$ *interactions*		
		-66.0 -11.3 -9.3	
$\{(Me_2Sn)_4O_5Cl_5\}\ldots\{Sn@3Me_2\}$	-705.1	-254.2	-450.8
	Decomposed $\boldsymbol{E_{orb}}$ *interactions*		
		-74.2 -43.7 -20.0 -14.0 -10.7 -10.9	
$\{(Me_2Sn)_4O_5Cl_4\}\ldots\{Sn@2ClMe_2\}$	-313.5	-176.8	-136.7
	Decomposed $\boldsymbol{E_{orb}}$ *interactions*		
		-78.4 -30.9 -11.6	

Table S10. Second order perturbation theory calculated strength of donor acceptor interaction ($n \rightarrow \sigma^*$) in $\{(Ete_2Sn)_5O_3Cl_5\}$ unit of complex **2b** along with details of corresponding lone pair and antibonding orbital with its occupancy.

Molecule	*Donor*	Acceptor M-L* type	Occupancy (M-L*)	ΔE_{M-L^*} (kcal/mole)
$[\{(Et_2Sn)_5O_3Cl_5\}] \}$	n_O(LP)	σ*(Sn-Cl)	0.218	47.1
	n_O (LP)	σ*(Sn-Cl)	0.216	41.7
	n_O (LP)	σ*(Sn-Cl)	0.154	32.3
	n_O (LP)	σ*(Sn-O)	0.138	20.7
	n_O (LP)	σ*(Sn-O)	0.161	18.3
	n_O (LP)	σ*(Sn-O)	0.158	18.8
	n_{Cl} (LP)	σ*(SnCl)	0.153	24.9

Table S11. NBO computed NPA charges on DFT optimized geometry of [{PtCl(SeC_5H_4N)(dppp)}] fragment of complex **2b**.

[{PtCl (SeC_5H_4N)(dppp)}]	
Pt 1	**0.11302**
P 2	**1.05853**
P 3	**1.03011**
Se 4	**-0.10529**
Cl 5	**-0.49317**
N 6	**-0.54813**
C 7	-0.34010
C 8	-0.22528
H 9	0.25674
C 10	-0.22507
H 11	0.24526
C 12	-0.22626
H 13	0.24214
C 14	-0.22762
H 15	0.24237
C 16	-0.22127
H 17	0.25087
C 18	-0.36214
C 19	-0.19842
H 20	0.26962
C 21	-0.23246
H 22	0.24667
C 23	-0.22666
H 24	0.24117
C 25	-0.23303
H 26	0.24208
C 27	-0.22433
H 28	0.23490
C 29	-0.75946
H 30	0.27528
H 31	0.27093
C 32	-0.47401
H 33	0.24746
H 34	0.25631
C 35	-0.74837
H 36	0.26690
H 37	0.27213
C 38	-0.36579
C 39	-0.23876
H 40	0.24062
C 41	-0.23968
H 42	0.24151
C 43	-0.21981
H 44	0.24084
C 45	-0.22722
H 46	0.24554
C 47	-0.20927
H 48	0.28234
C 49	-0.33700
C 50	-0.21969
H 51	0.24976
C 52	-0.23188
H 53	0.24110
C 54	-0.22528
H 55	0.24077

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C 56	-0.22843
H 57	0.24313
C 58	-0.20564
H 59	0.25210
C 60	-0.27795
H 61	0.24977
C 62	-0.20287
H 63	0.24087
C 64	-0.30198
H 65	0.24006
C 66	0.04743
H 67	0.21386
C 68	0.07016

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DFT optimized geometries

[{Pt(κ$_2$-SeC$_5$H$_4$N)(dppp)}] unit of complex 2a

E_{SCF} = -4495.39087860 Eh

G = -4494.93057201 Eh

Pt	8.660687000000	2.061076000000	3.564174000000
Se	10.874042000000	3.230703000000	3.613252000000
P	8.980038000000	0.779256000000	5.403547000000
P	6.571942000000	1.162657000000	3.315585000000
N	8.889371000000	3.227011000000	1.806942000000
C	10.131585000000	3.778197000000	1.944099000000
C	10.680488000000	4.590407000000	0.938527000000
H	11.679586000000	5.027583000000	1.073588000000
C	9.928514000000	4.809021000000	-0.222826000000
H	10.333380000000	5.440772000000	-1.028047000000
C	8.660396000000	4.211259000000	-0.361255000000
H	8.053379000000	4.356100000000	-1.265031000000
C	8.169993000000	3.418793000000	0.681057000000
H	7.188764000000	2.928953000000	0.630032000000
C	10.305804000000	1.390854000000	6.499224000000
C	10.286670000000	2.750312000000	6.883410000000
H	9.507780000000	3.424815000000	6.494786000000
C	11.277697000000	3.245115000000	7.743419000000
H	11.264441000000	4.304793000000	8.038412000000
C	12.290745000000	2.391869000000	8.214639000000
H	13.072385000000	2.784534000000	8.882061000000
C	12.310703000000	1.040795000000	7.830302000000
H	13.105467000000	0.373914000000	8.196485000000
C	11.319445000000	0.534348000000	6.974552000000
H	11.338834000000	-0.522920000000	6.671785000000
C	9.489786000000	-0.882887000000	4.849126000000
C	10.550301000000	-0.951993000000	3.916044000000
H	11.045234000000	-0.026192000000	3.580895000000
C	10.962898000000	-2.194436000000	3.417643000000
H	11.795361000000	-2.244615000000	2.699955000000
C	10.309315000000	-3.370906000000	3.826586000000
H	10.626425000000	-4.344906000000	3.424732000000
C	9.254937000000	-3.304115000000	4.750768000000
H	8.744914000000	-4.222963000000	5.075646000000
C	8.849986000000	-2.064169000000	5.271508000000
H	8.034363000000	-2.032440000000	6.006994000000
C	7.543306000000	0.594791000000	6.554198000000
H	7.867625000000	-0.097446000000	7.358839000000
H	7.449857000000	1.595325000000	7.027529000000
C	6.200160000000	0.153266000000	5.954998000000
H	6.283947000000	-0.866986000000	5.527733000000
H	5.472332000000	0.073612000000	6.789502000000
C	5.608552000000	1.094608000000	4.898016000000

H	5.554574000000	2.139516000000	5.269287000000
H	4.571737000000	0.795026000000	4.642868000000
C	6.609273000000	-0.552328000000	2.693781000000
C	7.766416000000	-0.992263000000	2.016988000000
H	8.603723000000	-0.292423000000	1.871205000000
C	7.853499000000	-2.314823000000	1.560505000000
H	8.760527000000	-2.652707000000	1.039043000000
C	6.790552000000	-3.205928000000	1.782627000000
H	6.862982000000	-4.246719000000	1.433012000000
C	5.632303000000	-2.770807000000	2.450142000000
H	4.797023000000	-3.467029000000	2.618007000000
C	5.536546000000	-1.446261000000	2.903361000000
H	4.621194000000	-1.115553000000	3.417094000000
C	5.497215000000	2.127015000000	2.199285000000
C	4.933735000000	1.560990000000	1.037552000000
H	5.098453000000	0.498131000000	0.806075000000
C	4.172741000000	2.364919000000	0.171946000000
H	3.735220000000	1.924220000000	-0.736371000000
C	3.970562000000	3.724319000000	0.463813000000
H	3.374885000000	4.349917000000	-0.217713000000
C	4.530706000000	4.288133000000	1.624769000000
H	4.376981000000	5.353713000000	1.851237000000
C	5.298328000000	3.495723000000	2.489361000000
H	5.769673000000	3.948021000000	3.376506000000

{$Me_{10}Sn_5(\mu\text{-}O)_3(\mu\text{-}Cl)Cl_4$} unit of complex 2a

E_{SCF} = -3998.50308706 Eh

G = -3998.21294200 Eh

Sn	3.539601000000	9.465115000000	7.349425000000
Sn	5.529300000000	6.348476000000	6.387937000000
Sn	6.858948000000	9.403912000000	5.813783000000
Sn	8.767952000000	6.879965000000	4.492600000000
Sn	10.026890000000	10.055910000000	3.507978000000
Cl	2.413090000000	7.233159000000	7.877523000000
Cl	4.958150000000	11.589076000000	6.728332000000
Cl	6.841445000000	4.280972000000	5.522554000000
Cl	10.947532000000	7.521708000000	2.867810000000
Cl	8.957680000000	12.131343000000	4.347821000000
O	5.190693000000	8.471176000000	6.782016000000
O	7.214103000000	7.334962000000	5.786761000000
O	8.840710000000	8.928028000000	4.656337000000
C	2.166563000000	9.856383000000	5.744286000000
H	2.302257000000	10.891421000000	5.383148000000
H	1.133438000000	9.678339000000	6.095533000000
H	2.404042000000	9.133619000000	4.941006000000
C	3.533863000000	10.086894000000	9.403397000000
H	4.540445000000	9.860894000000	9.803051000000
H	2.766817000000	9.518767000000	9.959696000000
H	3.358240000000	11.176882000000	9.455341000000

C	4.089221000000	6.258509000000	4.806839000000
H	3.093758000000	6.484656000000	5.230251000000
H	4.113225000000	5.260485000000	4.334943000000
H	4.378698000000	7.037383000000	4.075819000000
C	5.669937000000	5.760635000000	8.433740000000
H	4.868276000000	6.268624000000	8.998164000000
H	6.669261000000	6.083310000000	8.782018000000
H	5.581256000000	4.662296000000	8.509233000000
C	5.979333000000	9.866522000000	3.925628000000
H	4.892333000000	10.004723000000	4.057867000000
H	6.193495000000	9.024021000000	3.241552000000
H	6.441339000000	10.797052000000	3.549962000000
C	8.014615000000	10.154849000000	7.430557000000
H	7.344642000000	10.342231000000	8.287363000000
H	8.496822000000	11.091189000000	7.098163000000
H	8.775741000000	9.389221000000	7.668925000000
C	7.730716000000	6.336478000000	2.706026000000
H	7.802559000000	7.188022000000	2.004672000000
H	6.681733000000	6.110949000000	2.967388000000
H	8.208348000000	5.445684000000	2.260232000000
C	10.124449000000	5.911439000000	5.820498000000
H	9.525923000000	5.330863000000	6.544850000000
H	10.710302000000	6.702592000000	6.324345000000
H	10.800680000000	5.252982000000	5.246989000000
C	9.326860000000	10.246915000000	1.488077000000
H	9.440191000000	11.296733000000	1.160303000000
H	8.252454000000	9.983353000000	1.500386000000
H	9.880857000000	9.552500000000	0.831868000000
C	11.979265000000	10.420364000000	4.316850000000
H	12.080610000000	11.494614000000	4.555458000000
H	12.745962000000	10.089831000000	3.592662000000
H	12.062206000000	9.812961000000	5.237275000000

{$Et_{10}Sn_5(\mu\text{-}O)_3(\mu\text{-}Cl)Cl_4$} unit of complex 2b

E_{SCF} = -4391.37982848 Eh

G = -4390.81738641 Eh

Sn	9.910206000000	5.135761000000	12.060805000000
Sn	9.359110000000	8.806060000000	12.675273000000
Sn	6.609699000000	6.857328000000	12.195383000000
Sn	5.799740000000	10.103569000000	12.896733000000
Sn	2.890099000000	8.039316000000	12.560537000000
Cl	7.644800000000	3.869648000000	11.880022000000
Cl	11.955635000000	6.702918000000	12.394384000000
Cl	8.807318000000	11.359533000000	13.148181000000
Cl	3.045651000000	10.676022000000	13.352411000000
Cl	3.219490000000	5.694573000000	11.782920000000
O	8.761203000000	6.746772000000	12.386309000000
O	7.329682000000	8.805785000000	12.400341000000

O	4.852488000000	8.359743000000	12.325116000000
C	10.339000000000	4.909317000000	9.949332000000
H	9.513841000000	4.292406000000	9.542941000000
H	10.233090000000	5.936980000000	9.545192000000
C	11.721205000000	4.327979000000	9.654014000000
H	11.925083000000	4.292129000000	8.560801000000
H	11.822396000000	3.290190000000	10.036646000000
H	12.519148000000	4.937538000000	10.125362000000
C	10.544865000000	3.887001000000	13.722446000000
H	9.727380000000	3.150913000000	13.849238000000
H	11.435897000000	3.349223000000	13.335422000000
C	10.870405000000	4.642331000000	15.009005000000
H	11.644880000000	5.415308000000	14.833067000000
H	11.246854000000	3.951266000000	15.795439000000
H	9.976222000000	5.151528000000	15.420774000000
C	9.983321000000	8.560053000000	14.722175000000
H	9.098832000000	8.861755000000	15.319479000000
H	10.140016000000	7.472050000000	14.841834000000
C	11.225279000000	9.369846000000	15.084764000000
H	11.487631000000	9.247845000000	16.158812000000
H	11.066565000000	10.451703000000	14.897909000000
H	12.101040000000	9.037898000000	14.490077000000
C	10.205778000000	9.231455000000	10.740729000000
H	10.959168000000	10.028379000000	10.896648000000
H	10.740738000000	8.308732000000	10.446651000000
C	9.125809000000	9.646399000000	9.744838000000
H	9.561271000000	9.872769000000	8.746911000000
H	8.586521000000	10.551924000000	10.088844000000
H	8.368739000000	8.849192000000	9.604224000000
C	6.380241000000	6.502027000000	10.087402000000
H	7.423376000000	6.391857000000	9.729048000000
H	5.892928000000	5.512726000000	10.007533000000
C	5.616296000000	7.593626000000	9.346637000000
H	5.582971000000	7.385682000000	8.254632000000
H	6.084014000000	8.589830000000	9.480814000000
H	4.572740000000	7.668120000000	9.708658000000
C	6.037035000000	6.146208000000	14.148396000000
H	5.498626000000	7.010137000000	14.585881000000
H	5.295673000000	5.346682000000	13.957550000000
C	7.191835000000	5.678037000000	15.024848000000
H	6.830998000000	5.362929000000	16.028441000000
H	7.946149000000	6.475399000000	15.176190000000
H	7.706661000000	4.811446000000	14.565761000000
C	5.989733000000	10.150880000000	15.041895000000
H	5.183075000000	9.488830000000	15.415604000000
H	6.966749000000	9.668896000000	15.242841000000
C	5.907352000000	11.554865000000	15.635879000000
H	6.000536000000	11.532013000000	16.743931000000
H	4.937548000000	12.036416000000	15.393688000000
H	6.724540000000	12.195936000000	15.246650000000

C	5.784997000000	11.555687000000	11.307634000000
H	5.694080000000	12.541666000000	11.804811000000
H	6.808982000000	11.489354000000	10.892648000000
C	4.694659000000	11.332324000000	10.263151000000
H	4.749271000000	12.098814000000	9.459247000000
H	3.686786000000	11.389522000000	10.720542000000
H	4.786603000000	10.338968000000	9.780590000000
C	1.685140000000	8.762096000000	10.908905000000
H	0.937252000000	9.431030000000	11.380284000000
H	2.387357000000	9.415030000000	10.353509000000
C	1.053858000000	7.697150000000	10.016245000000
H	0.482222000000	8.163656000000	9.183443000000
H	0.353576000000	7.044854000000	10.577303000000
H	1.818638000000	7.028931000000	9.573829000000
C	2.326586000000	7.640785000000	14.618195000000
H	3.151299000000	8.105598000000	15.195627000000
H	1.431482000000	8.271863000000	14.793091000000
C	2.104065000000	6.178548000000	14.992842000000
H	1.834324000000	6.079907000000	16.067704000000
H	3.011393000000	5.569284000000	14.813936000000
H	1.291562000000	5.714776000000	14.397708000000

[{PtCl(SeC$_5$H$_4$N)(dppp)}] unit of complex 2b

E_{SCF} = -4955.85449364 Eh

G = -4955.39780556 Eh

Pt	4.919413000000	16.410809000000	5.049215000000
P	4.644988000000	15.896186000000	2.881490000000
P	2.818147000000	17.289685000000	5.145800000000
Se	7.031896000000	15.046752000000	5.052592000000
Cl	5.288401000000	16.933717000000	7.321049000000
N	5.070123000000	13.560323000000	6.445450000000
C	6.189837000000	15.783122000000	1.898786000000
C	7.201930000000	16.736567000000	2.138866000000
H	7.069559000000	17.478830000000	2.943307000000
C	8.380878000000	16.711415000000	1.381084000000
H	9.173360000000	17.448657000000	1.579937000000
C	8.556661000000	15.735331000000	0.384046000000
H	9.487557000000	15.709634000000	-0.202759000000
C	7.548255000000	14.787624000000	0.143597000000
H	7.686981000000	14.018522000000	-0.631671000000
C	6.362481000000	14.810559000000	0.896099000000
H	5.577469000000	14.060100000000	0.718359000000
C	3.791387000000	14.291263000000	2.647200000000
C	4.347870000000	13.164778000000	3.292639000000
H	5.285509000000	13.280573000000	3.857836000000
C	3.697927000000	11.926061000000	3.224008000000
H	4.138660000000	11.056174000000	3.734084000000
C	2.482768000000	11.800936000000	2.527682000000

H	1.964312000000	10.830492000000	2.490364000000
C	1.928296000000	12.917779000000	1.882797000000
H	0.976339000000	12.827565000000	1.338208000000
C	2.583721000000	14.158681000000	1.933585000000
H	2.136340000000	15.020142000000	1.419443000000
C	3.715490000000	17.144278000000	1.859841000000
H	4.424273000000	17.996784000000	1.791070000000
H	3.637012000000	16.724137000000	0.835254000000
C	2.345714000000	17.632863000000	2.352867000000
H	1.628941000000	16.787384000000	2.402058000000
H	1.942341000000	18.327735000000	1.585004000000
C	2.344032000000	18.361241000000	3.702335000000
H	1.342699000000	18.791205000000	3.909753000000
H	3.062655000000	19.207710000000	3.708465000000
C	1.616171000000	15.904125000000	5.082921000000
C	0.279245000000	16.093841000000	4.670798000000
H	-0.093622000000	17.101868000000	4.431816000000
C	-0.586299000000	14.994214000000	4.562672000000
H	-1.626216000000	15.146267000000	4.235039000000
C	-0.123079000000	13.703044000000	4.870175000000
H	-0.799990000000	12.840056000000	4.775018000000
C	1.202727000000	13.515114000000	5.292452000000
H	1.572913000000	12.505112000000	5.521412000000
C	2.077420000000	14.607546000000	5.398636000000
H	3.131907000000	14.453296000000	5.699864000000
C	2.351998000000	18.330468000000	6.573792000000
C	1.247294000000	18.028727000000	7.391944000000
H	0.646826000000	17.128084000000	7.196883000000
C	0.923522000000	18.873361000000	8.466989000000
H	0.062467000000	18.631793000000	9.108826000000
C	1.698284000000	20.015148000000	8.725998000000
H	1.444421000000	20.672940000000	9.571351000000
C	2.809854000000	20.308780000000	7.916134000000
H	3.433531000000	21.189612000000	8.131305000000
C	3.145307000000	19.464357000000	6.849537000000
H	4.043772000000	19.664375000000	6.246047000000
C	7.338396000000	13.003303000000	7.070038000000
H	8.414526000000	13.195665000000	6.950224000000
C	6.868761000000	12.042451000000	7.969467000000
H	7.579439000000	11.451539000000	8.568591000000
C	5.480345000000	11.856418000000	8.114869000000
H	5.068277000000	11.121806000000	8.822161000000
C	4.631806000000	12.647887000000	7.328343000000
H	3.534059000000	12.546466000000	7.411367000000
C	6.398743000000	13.753171000000	6.320146000000

Supplementary Information

$[SnCl_2(CH_3)_2]$ complex

E_{SCF} = -1214.48235559 Eh

G = -1214.44720980 Eh

Cl	2.291009449009	1.864507083967	3.943268424108
Sn	4.331415782309	1.925017971268	2.709764033067
Cl	6.096384395913	1.926106112793	4.313790491339
C	4.467219602733	0.067137912128	1.612438953779
H	5.423323623064	0.043205546707	1.055769491053
H	4.430979976547	-0.766480256900	2.337895536192
H	3.613267332190	-0.003084727202	0.912167509350
C	4.400819794029	3.826812977834	1.683798936695
H	5.356916045330	3.906894558143	1.132376615985
H	3.546897079173	3.891613743221	0.982959546718
H	4.331764919704	4.630769078041	2.439704461713