Electronic Supplementary Material (ESI) for RSC Advances.

Palladium(II) complexes with chiral organoantimony(III) ligands. Solution behaviour and solid state structures

Dana Copolovici,[a] Francesco Isaia,[b] Hans J. Breunig,[c] Ciprian I. Raț*[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: ciprian.rat@ubbcluj.ro, cristian.silvestru@ubbcluj.ro; Fax: (+40) 264-590818; Tel: (+40) 264-593833*
[b] *Dipartimento di Scienze Chimiche e Geologiche, Università degli Studi di Cagliari, S.S. 554 Bivio per Sestu, 09042 Monserrato (CA), Italy. E-mail: isaia@unica.it*
[c] *Institut für Anorganische und Physikalische Chemie, Universität Bremen, 28334 Bremen, Germany. E-mail: hbreunig@uni-bremen.de*

(2-$Me_2NCH_2C_6H_4$)PhSbCl (1)

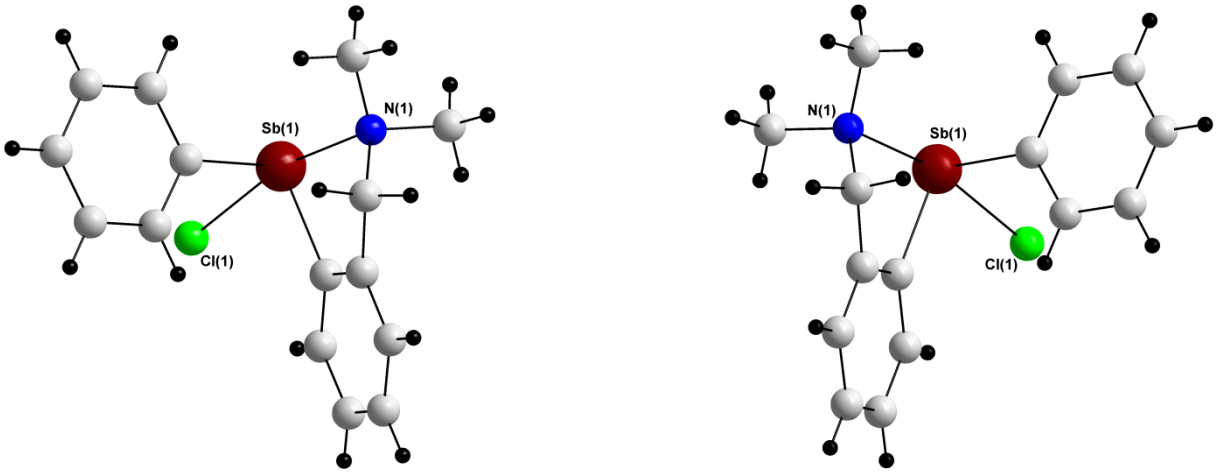

Fig. S1 Molecular structure of (R_N,A_{Sb}) [or (R_N,S_{Sb})] (*left*) and (S_N,C_{Sb}) [or (S_N,R_{Sb})] (*right*) isomers of **1**.

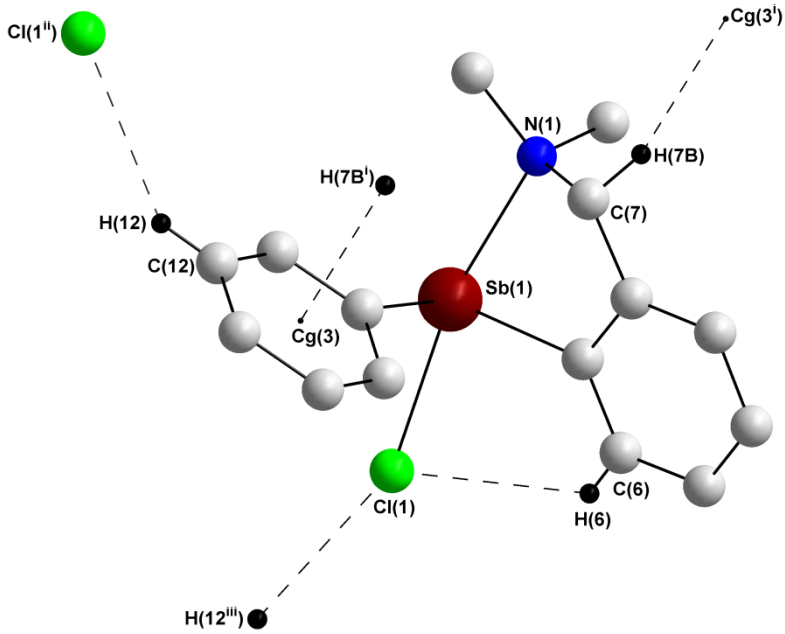

Fig. S2 Intramolecular and intermolecular C–H···Cl and C–H···Cg interactions in the crystal of **1** [Cg is the centroid of the phenyl ring C(10)–C(15)]. Symmetry codes: *(i)* 1–x, –y, 2–z; *(ii)* 1/2–x, –1/2+y, 3/2–z; *(iii)* 1/2–x, 1/2+y, 3/2–z.

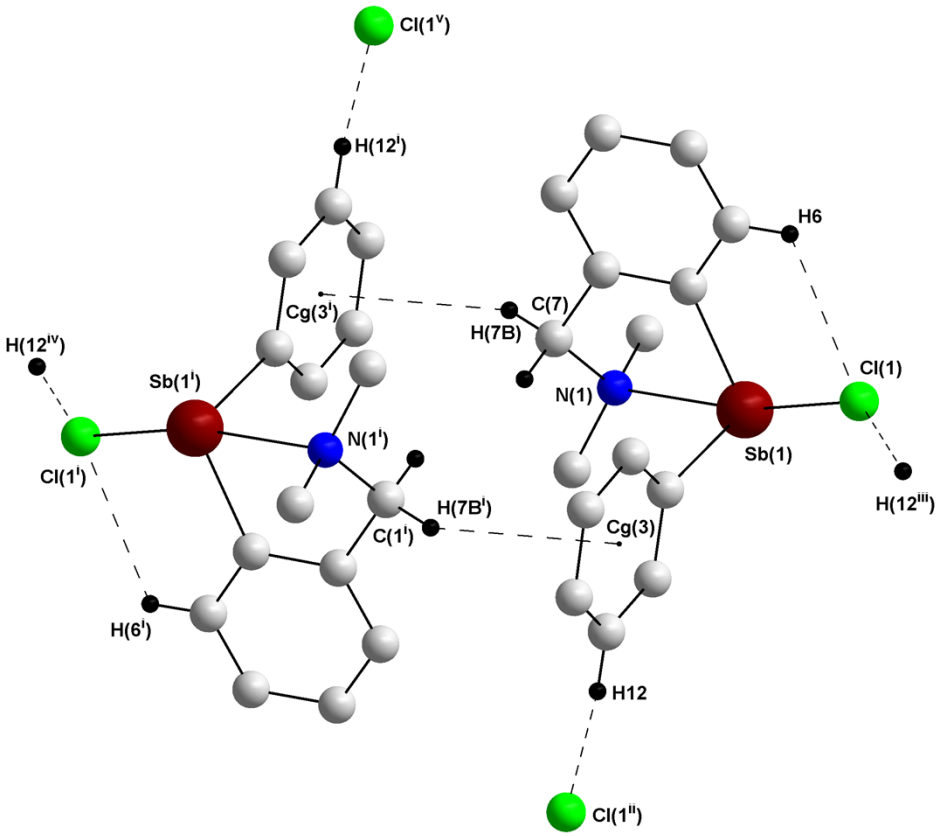

Fig. S3 Dimer association of (R_N,A_{Sb})-**1** and (S_N,C_{Sb})-**1** isomers in the layer structure of **1**. Symmetry codes: *(i)* 1–x, –y, 2–z; *(ii)* 1/2–x, –1/2+y, 3/2–z; *(iii)* 1/2–x, 1/2+y, 3/2–z; *(iv)* 1/2+x, –1/2–y, 1/2+z; *(v)* 1/2+x, 1/2–y, 1/2+z.

Table S1 Bond lengths and interatomic distances (Å) and angles (°) for intramolecular and intermolecular C–H···Cl and C–H···Cg interactions in the crystals of **1**.

D–H···A	***D–H***	***A···H***	***D···A***	***D–H···A***
C(6)–H(6)···Cl(1)	0.93	2.74	3.327(3)	122
C(12)–H(12)···Cl(1^{ii})	0.93	2.80	3.594(4)	144
C(7)–H(7B)···Cg(3^{i})	0.97	2.97	3.839(4)	149

Symmetry codes: *(i)* 1–x, –y, 2–z; *(ii)* 1/2–x, –1/2+y, 3/2–z.

(2-$Me_2NCH_2C_6H_4$)Mes_2Sb (2)

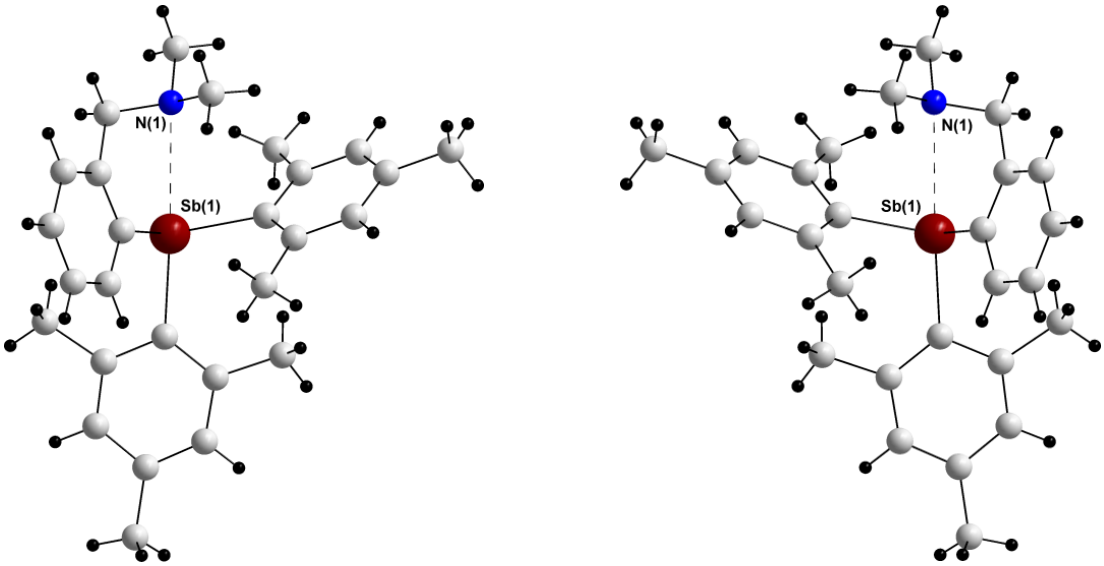

Fig. S4 Molecular structure of the (R_N,C_{Sb}) (*left*) and of the (S_N,A_{Sb}) (*right*) isomers of **2**.

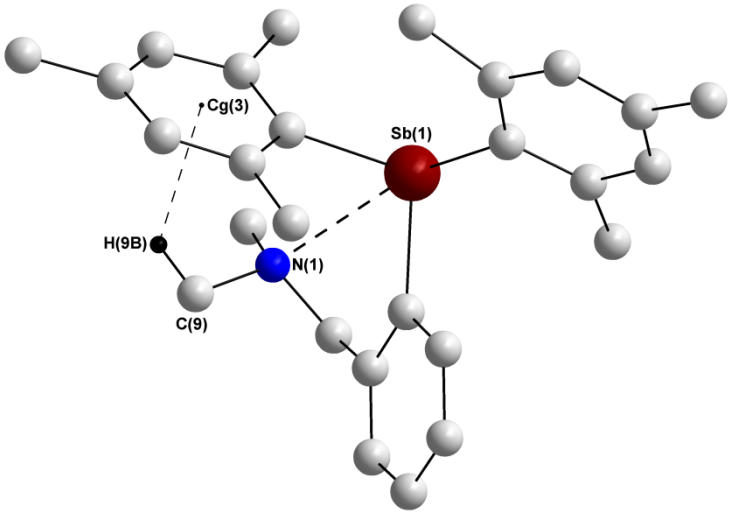

Fig. S5 Intramolecular C–H···Cg interactions in the crystal structure of **2** [Cg(3) is the centroid of the benzene ring C(19)–C(24)].

Table S2 Bond lengths and interatomic distances (Å) and angles (°) for intramolecular C–H···Cg interactions in the crystals of **2**.

D–H···A	***D–H***	***A···H***	***D···A***	***D–H···A***
C(9)–H(9B)···Cg(3)	0.97	2.92	3.546(5)	124

$[Me_2NHCH_2C_6H_5]^+[PdCl_3\{SbCl(Ph)(C_6H_4CH_2NMe_2\text{-}2)\text{-}Sb\}]^-$ (3)

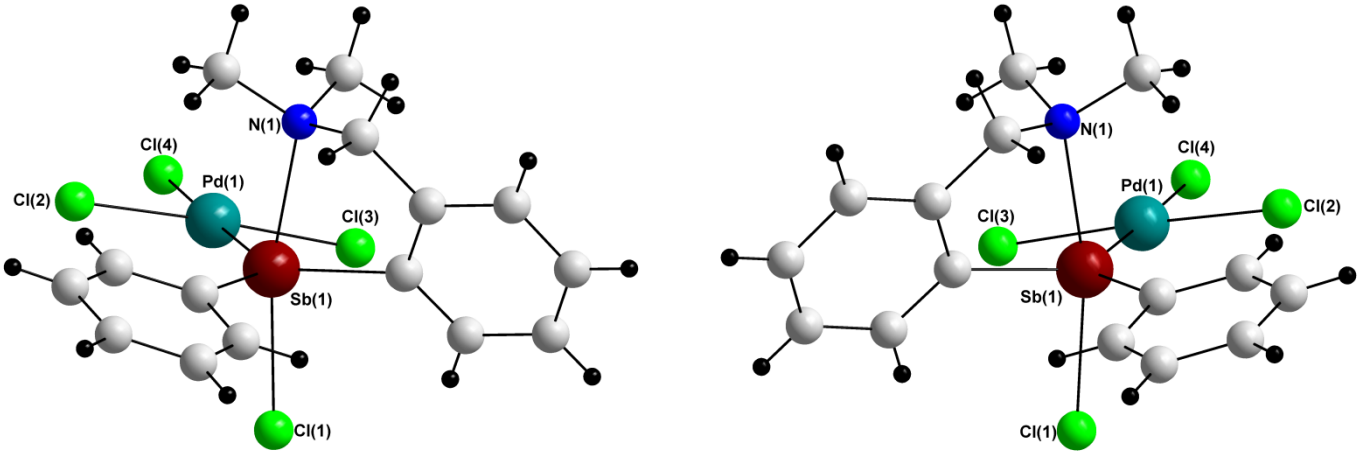

Fig. S6 Structure of (R_N,A_{Sb}) (*left*) and (S_N,C_{Sb}) (*right*) anions in the crystal structure of **3**.

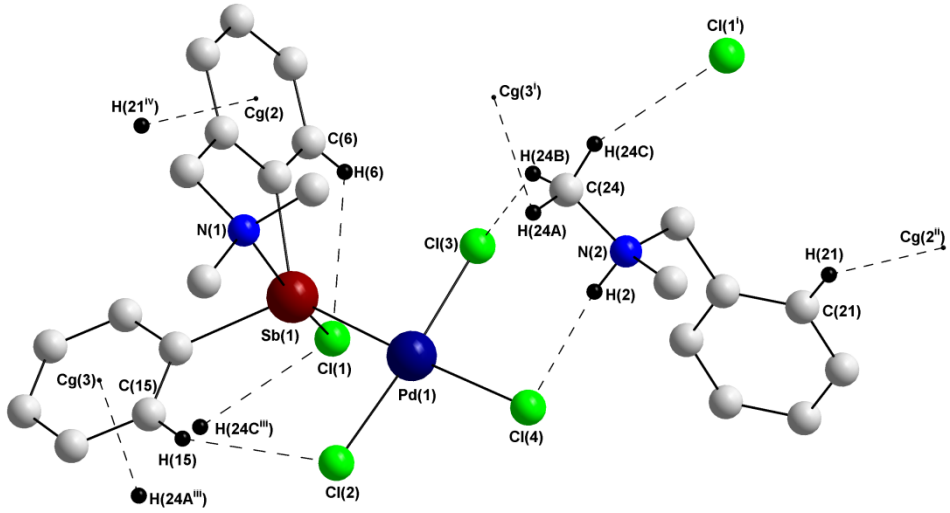

Fig. S7 Intramolecular and intermolecular C–H···Cl and C–H···Cg interactions in the crystal structure of **3** [Cg(2) and Cg(3) are the centroids of the benzene rings C(1)–C(6) and C(10)–C(15), respectively]. Symmetry codes: *(i)* x, –1+y, z; *(ii)* –1+x, –1+y, z; *(iii)* x, 1+y, z; (iv) 1+x, 1+y, z.

Table S3 Bond lengths and interatomic distances (Å) and angles (°) for intermolecular and intermolecular C–H···Cl and C–H···Cg interactions in the crystals of **3**.

D–H···A	***D–H***	***A···H***	***D···A***	***D–H···A***
N(2)–H(2)···Cl(4)	0.87(6)	2.25(6)	3.111(8)	171(8)
C(6)–H(6)···Cl(1)	0.93	2.78	3.333(9)	119
C(15)–H(15)···Cl(2)	0.93	2.70	3.511(10)	146
C(24)–H(24B)···Cl(3)	0.96	2.69	3.432(11)	135
C(24)–H(24C)···Cl(1^i)	0.96	2.73	3.624(11)	156
C(21)–H(21)···Cg(2^{iv})	0.93	3.00	3.848(11)	153
C(24)–H(24A)···Cg(3^i)	0.96	2.95	3.443(12)	113

Symmetry codes: *(i)* x, –1+y, z; *(ii)* –1+x, –1+y, z; *(iii)* x, 1+y, z; *(iv)* 1+x, 1+y, z.

[$PdCl_2${$SbMes_2(C_6H_4CH_2NMe_2$-2)-*N*,*Sb*}] (4)

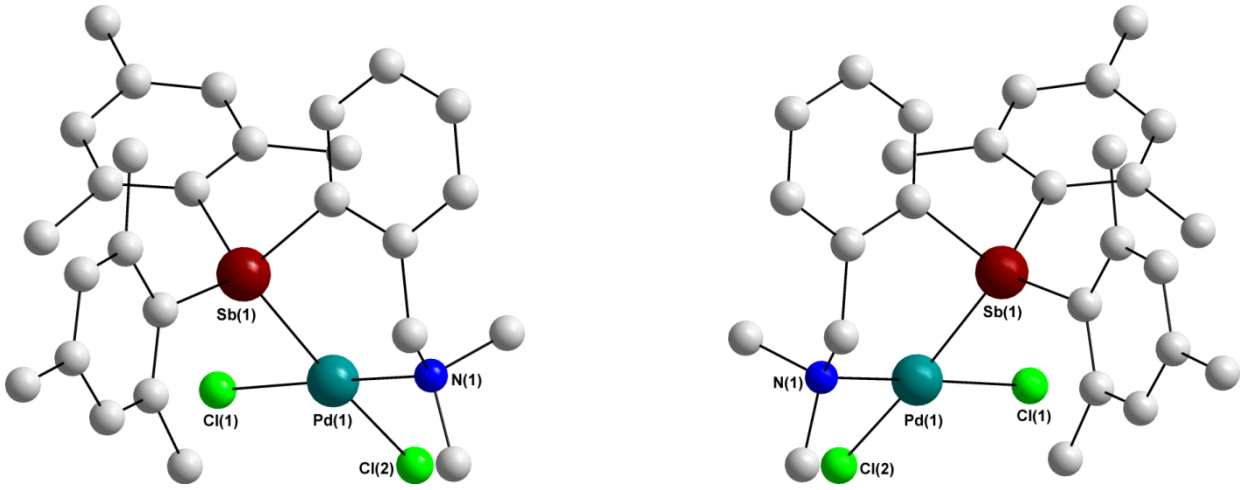

Fig. S8 Molecular structure of (S_N) (*left*) and (R_N) (*right*) isomers in the crystal structure of **4**. The hydrogen atoms were omitted for clarity.

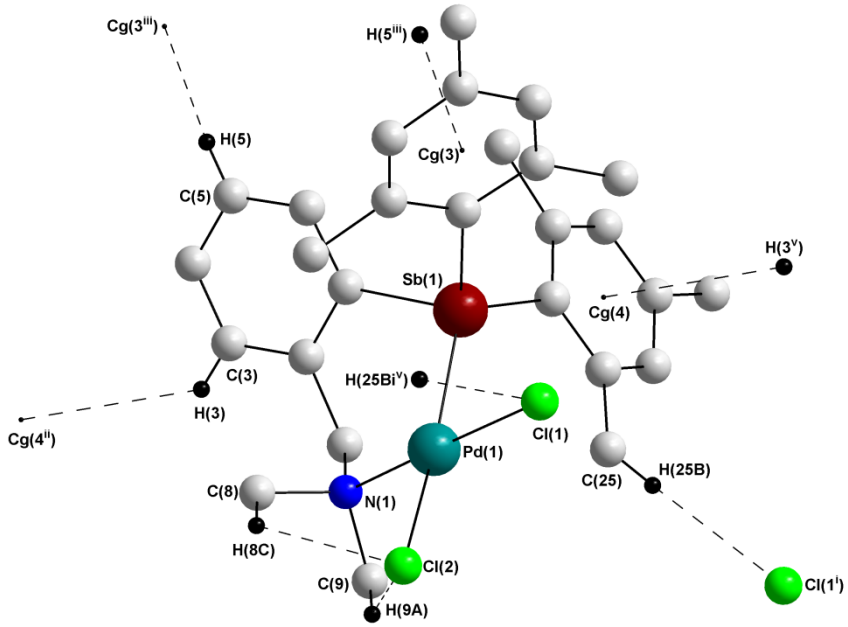

Fig. S9 Intramolecular and intermolecular C–H···Cl and C–H···Cg interactions in the crystal structure of **4** [Cg(3) and Cg(4) are the centroids of the benzene rings C(10)–C(15) and C(19)–C(24), respectively]. Symmetry codes: *(i)* 1/2+x,1/2–y,1/2+z; *(ii)* –1+x, y, z; *(iii)* –x, –y, –z; *(iv)* –1/2+x, 1/2–y, –1/2+z; *(v)* 1+x, y, z.

Table S4 Bond lengths and interatomic distances (Å) and angles (°) for intramolecular and intermolecular C–H···Cl and C–H···Cg interactions in the crystals of **4**.

D–H···A	***D–H***	***A···H***	***D···A***	***D–H···A***
C(9)–H(9A)···Cl(2)	0.96	2.61	3.303(5)	129
C(25)–H(25B)···Cl(1^{i})	0.96	2.73	3.686(6)	177
C(3)–H(3)···Cg(4)		2.98	3.681(6)	133
C(5)–H(5)···Cg(3)		2.68	3.428(5)	138

Symmetry codes: (i) 1/2+x,1/2–y,1/2+z; (ii) –1+x, y, z; (iii) –x, –y, –z

Table S5 Comparison of selected bond lengths (Å) and angles (°) of the calculated and determined molecular structure of **1**.

	X-ray	DFT	Abs. err. (%)	Rel. err. (%)
Sb(1)−C(1)	2.147	2.18464	–0.04	1.7
Sb(1)−C(10)	2.153	2.17348	–0.02	0.9
Sb(1)−Cl(1)	2.5111	2.47450	0.04	1.5
Sb(1)−N(1)	2.452	2.66287	–0.21	7.9
C(1)−Sb(1)−C(10)	94.98	94.749	0.23	0.2
C(1)−Sb(1)−Cl(1)	91.00	92.681	–1.68	1.8
C(10)−Sb(1)−Cl(1)	88.54	92.467	–3.93	4.2
C(1)−Sb(1)−N(1)	74.59	72.291	2.30	3.2
C(10)−Sb(1)−N(1)	88.78	82.739	6.04	7.3
Cl(1)−Sb(1)−N(1)	165.05	163.680	1.37	0.8

Table S6 Comparison of selected bond lengths (Å) and angles (°) of the calculated and determined molecular structure of **2**.

	X-ray	DFT	Abs. err. (%)	Rel err. (%)
Sb(1)−C(1)	2.172	2.19776	–0.03	1.2
Sb(1)−C(10)	2.203	2.21391	–0.01	0.5
Sb(1)−C(19)	2.178	2.19734	–0.02	0.9
Sb(1)−N(1)	3.052	3.02215	0.03	1.0
C(1)−Sb(1)−C(19)	100.95	100.557	0.39	0.4
C(1)−Sb(1)−C(10)	96.06	95.235	0.83	0.9
C(10)−Sb(1)−C(19)	104.88	103.260	1.62	1.6
C(1)−Sb(1)−N(1)	67.54	68.342	–0.80	1.2
C(10)−Sb(1)−N(1)	162.4	160.589	1.81	1.1
C(19)−Sb(1)−N(1)	73.46	71.217	2.24	3.1

Table S7 Comparison of selected bond lengths (Å) and angles (°) of the calculated and determined molecular structure of the anion of **3**.

	X-ray	DFT	Abs. err. (%)	Rel. err. (%)
Sb(1)−C(1)	2,108	2,16299	–0,05	2,5
Sb(1)−C(10)	2,130	2,16371	–0,03	1,6
Sb(1)−Cl(1)	2,487	2,47082	0,02	0,7
Sb(1)−N(1)	2,385	2,63063	–0,25	9,3
Sb(1)−Pd(1)	2,4783	2,51671	–0,04	1,5
Pd(1)−Cl(2)	2,288	2,35167	–0,06	2,7
Pd(1)−Cl(3)	2,302	2,35155	–0,05	2,1
Pd(1)−Cl(4)	2,360	2,33178	0,03	1,2
C(1)−Sb(1)−C(10)	102,4	98,215	4,19	4,3
C(1)−Sb(1)−Cl(1)	91,40	92,772	–1,37	1,5
C(10)−Sb(1)−Cl(1)	91,10	91,186	–0,09	0,1
C(1)−Sb(1)−N(1)	76,00	72,492	3,51	4,8
C(10)−Sb(1)−N(1)	88,80	82,680	6,12	7,4
Cl(1)−Sb(1)−N(1)	167,05	162,919	4,13	2,5
Cl(1)−Sb(1)−Pd(1)	95,65	110,119	–14,47	13,1
N(1)−Sb(1)−Pd(1)	94,61	85,777	8,83	10,3
Cl(2)−Pd(1)−Sb(1)	90,88	92,212	–1,33	1,4
Cl(3)−Pd(1)−Sb(1)	83,76	82,293	1,47	1,8
Cl(4)−Pd(1)−Sb(1)	177,71	171,323	6,39	3,7
Cl(2)−Pd(1)−Cl(3)	174,36	174,119	0,24	0,1
Cl(2)−Pd(1)−Cl(4)	91,40	92,009	–0,61	0,7

Table S8 Comparison of selected bond lengths (Å) and angles (°) of the calculated and determined molecular structure of **4**.

	X-ray	DFT	Abs. err. (%)	Rel. err. (%)
Sb(1)−C(1)	2,131	2,15555	–0,02	1,1
Sb(1)−C(10)	2,133	2,14547	–0,01	0,6
Sb(1)−C(19)	2,147	2,16421	–0,02	0,8
Sb(1)−Pd(1)	2,4831	2,50603	–0,02	0,9
Pd(1)−Cl(1)	2,3029	2,31745	–0,01	0,6
Pd(1)−Cl(2)	2,3769	2,35913	0,02	0,8
Pd(1)−N(1)	2,133	2,21860	–0,09	3,9
C(1)−Sb(1)−C(10)	103,64	101,792	1,85	1,8
C(1)−Sb(1)−C(19)	100,23	101,082	–0,85	0,8
C(10)−Sb(1)−C(19)	115,40	110,783	4,62	4,2
Pd(1)−Sb(1)−C(1)	103,49	100,811	2,68	2,7
Pd(1)−Sb(1)−C(10)	110,42	122,066	–11,65	9,5
Pd(1)−Sb(1)−C(19)	120,68	115,997	4,68	4,0
Sb(1)−Pd(1)−Cl(1)	82,12	84,161	–2,04	2,4
Sb(1)−Pd(1)−Cl(2)	168,34	174,581	–6,24	3,6
Cl(1)−Pd(1)−Cl(2)	91,51	92,736	–1,23	1,3
Sb(1)−Pd(1)−N(1)	94,55	93,133	1,42	1,5
Cl(1)−Pd(1)−N(1)	173,96	175,888	–1,93	1,1

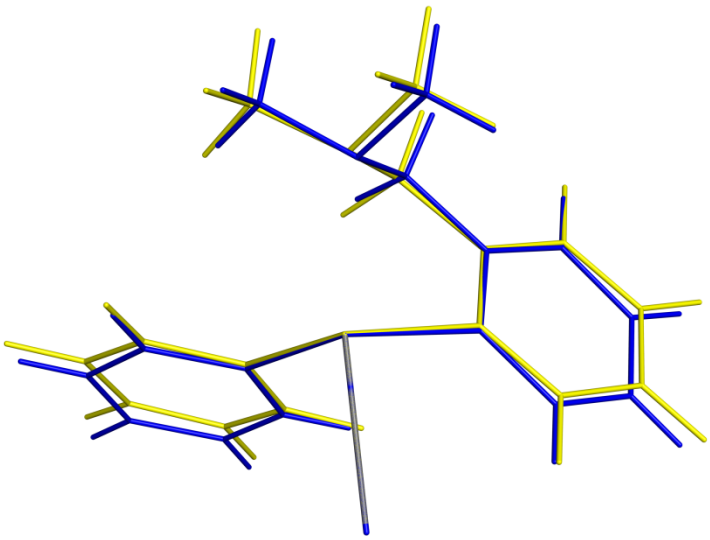

Fig. S10 Overlay of the calculated (yellow) and determined (blue) molecular structure of **1**.

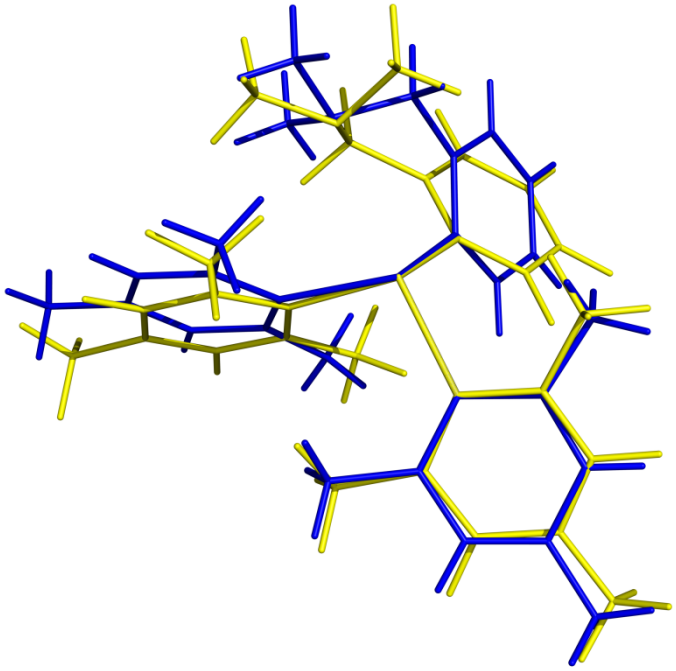

Fig. S11 Overlay of the calculated (yellow) and determined (blue) molecular structure of **2**.

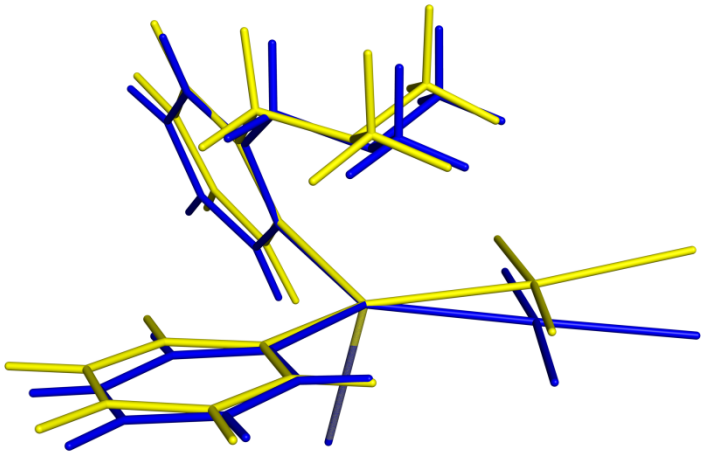

Fig. S12 Overlay of the calculated (yellow) and determined (blue) molecular structure of the anion of **3**.

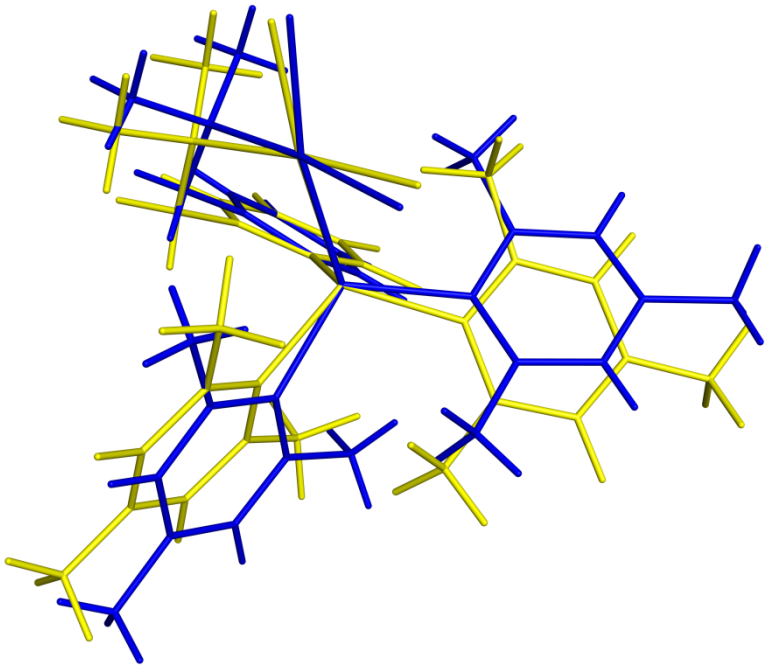

Fig. S13 Overlay of the calculated (yellow) and determined (blue) molecular structure of **4**.

Table S9 Cartesian coordinates (Å) of the optimized structure of 2-(Me_2NCH_2)C_6H_4(Ph)SbCl (**1**).

Atom	x	y	z
C	4.902212	5.955814	2.908917
C	6.134772	5.772701	3.585539
C	7.331975	5.700118	2.847091
H	8.284353	5.553841	3.375202
C	7.317612	5.817349	1.447111
H	8.257063	5.759923	0.883212
C	6.097780	6.002429	0.775854
H	6.077164	6.094331	-0.317458
C	4.896629	6.067879	1.505759
H	3.946458	6.227574	0.979322
C	6.161918	5.709840	5.099003
H	7.107875	5.249178	5.463432
H	6.123404	6.740872	5.502802
C	4.799939	5.222203	7.066911
H	5.644186	4.809273	7.661465
H	3.866951	4.736788	7.402525
H	4.719064	6.304419	7.262269
C	5.042589	3.552087	5.321902
H	5.887378	3.057896	5.849627
H	5.174924	3.404429	4.236814
H	4.099950	3.068595	5.630937
C	3.541203	7.824822	5.130944
C	4.444845	8.765892	4.594896
H	4.909334	8.582295	3.616733
C	4.754087	9.939510	5.304885
H	5.459513	10.664525	4.878761
C	4.157760	10.187959	6.554713
H	4.398660	11.105107	7.106830
C	3.244550	9.263096	7.089664
H	2.766619	9.457551	8.058466
C	2.937431	8.087936	6.378335
H	2.217825	7.376012	6.807497
Cl	1.818142	7.194439	2.312458
N	4.984261	4.992291	5.627247
Sb	3.057982	5.984908	4.079655

Table S10 Cartesian coordinates (Å) of the optimized structure of 2-(Me_2NCH_2)C_6H_4(Ph)SbCl, N atom not coordinated to Sb.

Atom	x	y	z
C	5.928153	7.042204	3.045771
C	5.967599	5.733810	3.584557
C	6.186080	4.639209	2.721883
H	6.236950	3.633381	3.158285
C	6.356684	4.835281	1.343056
H	6.529826	3.974313	0.685104
C	6.302405	6.134183	0.808682
H	6.434048	6.296221	-0.268729
C	6.085603	7.232898	1.658715
H	6.058716	8.246576	1.238224
C	5.752921	5.475846	5.067091
H	5.774091	6.458293	5.624486
H	4.729458	5.077880	5.220375
C	6.304843	4.112966	6.984742
H	6.331059	4.952700	7.722459
H	6.990769	3.325925	7.345511
H	5.281124	3.697070	6.974708
C	8.081070	4.985991	5.588716
H	8.269762	5.867562	6.243169
H	8.343146	5.273581	4.557073
H	8.751817	4.166668	5.902411
C	7.651728	8.548954	5.203917
C	8.731661	8.211487	4.362921
H	8.566736	8.075031	3.285905
C	10.015862	8.029876	4.902497
H	10.851989	7.762581	4.243863
C	10.228344	8.180012	6.285714
H	11.230339	8.029189	6.706553
C	9.158174	8.530204	7.127276
H	9.322521	8.655798	8.204984
C	7.873081	8.718012	6.585999
H	7.043299	8.987429	7.254831
Cl	6.164781	10.420517	2.790924
N	6.691934	4.523906	5.639635
Sb	5.639533	8.718157	4.415822

Table S11 Cartesian coordinates (Å) of the optimized structure of 2-(Me_2NCH_2)$C_6H_4SbMes_2$ (**2**).

Atom	x	y	z
C	0.009903	0.055999	-2.204162
C	-1.184394	0.322452	-2.922062
C	-1.158407	0.341034	-4.332532
H	-2.092860	0.528182	-4.879647
C	0.034449	0.126825	-5.040897
H	0.034202	0.145207	-6.138032
C	1.222942	-0.114647	-4.332292
H	2.165317	-0.283738	-4.869062
C	1.202268	-0.150375	-2.927597
H	2.137258	-0.349629	-2.386880
C	-2.488661	0.608592	-2.198093
H	-2.411541	1.589847	-1.685379
H	-3.320692	0.703318	-2.938531
C	-3.873919	0.005994	-0.293961
H	-3.629575	0.968200	0.191821

Table S12 Cartesian coordinates (Å) of the optimized structure of 2-(Me_2NCH_2)$C_6H_4SbMes_2$; N atom not coordinated to Sb.

Atom	x	y	z
C	-0.318255	0.907893	2.360147
C	-0.830385	2.042295	3.035874
C	-2.061979	2.596312	2.619809
H	-2.452337	3.459263	3.174891
C	-2.779549	2.046973	1.548291
H	-3.735684	2.490493	1.242578
C	-2.268947	0.924060	0.873576
H	-2.824401	0.475285	0.040018
C	-1.048738	0.362809	1.282531
H	-0.685421	-0.542492	0.777596
C	-0.100783	2.707823	4.194091
H	0.740865	2.054630	4.539152
H	0.373514	3.640338	3.826036
C	-1.570718	1.889383	5.948442
H	-0.814380	1.254473	6.463721

H	-4.009167	-0.756932	0.492915
H	-4.844509	0.122835	-0.833895
C	-3.016068	-1.723767	-1.745303
H	-3.935728	-1.753563	-2.377540
H	-3.112792	-2.463603	-0.932531
H	-2.155837	-2.017177	-2.369209
C	2.162264	0.060423	0.242617
C	2.861928	1.183473	-0.289860
C	4.268367	1.245654	-0.187529
H	4.791478	2.116048	-0.609978
C	5.014587	0.242134	0.450691
C	4.302346	-0.817283	1.041481
H	4.858941	-1.586128	1.597167
C	2.897287	-0.922830	0.968115
C	2.159311	2.348358	-0.963162
H	2.764851	3.268156	-0.885045
H	1.173706	2.561356	-0.507951
H	1.978164	2.157954	-2.037559
C	6.524816	0.296944	0.512016
H	6.975038	-0.348936	-0.266985
H	6.905613	-0.058261	1.486698
H	6.903607	1.321354	0.349284
C	2.249712	-2.072740	1.715375
H	1.919310	-2.882058	1.041172
H	1.353780	-1.755078	2.275508
H	2.958893	-2.511535	2.438603
C	-0.625642	-1.978562	0.419694
C	-0.288666	-3.103214	-0.380781
C	-0.907345	-4.344486	-0.120990
H	-0.640313	-5.207594	-0.748194
C	-1.848528	-4.515886	0.909595
C	-2.131787	-3.403154	1.720958
H	-2.833522	-3.518052	2.559616
C	-1.530151	-2.144894	1.504637
C	0.725849	-3.040896	-1.500988
H	0.277575	-2.661985	-2.437636
H	1.142363	-4.041664	-1.710565
H	1.564530	-2.366408	-1.256727
C	-2.518128	-5.853604	1.134445
H	-3.113642	-5.862082	2.063833
H	-1.775023	-6.669904	1.199703
H	-3.198762	-6.103773	0.298207
C	-1.837450	-1.031593	2.488795
H	-2.118698	-0.089031	1.987569
H	-0.955162	-0.802864	3.118591
H	-2.659570	-1.315250	3.168688
N	-2.781576	-0.397460	-1.173180
Sb	-0.037226	0.095026	-0.007254

Table S13 Cartesian coordinates (Å) of the optimized structure of [{2-(Me_2NCH_2)C_6H_4}(Ph)(Cl)SbPdCl_3]$^-$; anion of **3**.

Atom	x	y	z
C	5.360101	4.884780	3.003466
C	6.333688	5.524820	3.805071
C	7.618167	5.760248	3.276673
H	8.376245	6.251066	3.903297
C	7.936510	5.362862	1.967486
H	8.943058	5.546280	1.569272
C	6.970351	4.713481	1.179712
H	7.217694	4.382208	0.162876
C	5.686223	4.472856	1.699569
H	-2.076215	1.262313	5.194851
H	-2.322986	2.211664	6.690560
C	-0.300151	3.915658	6.273659
H	-1.006909	4.222315	7.065738
H	0.078196	4.829238	5.779780
H	0.564857	3.405917	6.767908
C	1.611761	-1.691210	1.688794
C	1.766130	-1.383448	0.303882
C	1.778494	-2.430991	-0.639669
H	1.888807	-2.182004	-1.704904
C	1.680759	-3.780751	-0.258140
C	1.628162	-4.064569	1.117422
H	1.616579	-5.114565	1.443885
C	1.610722	-3.052879	2.102196
C	1.976443	0.034078	-0.197374
H	1.072396	0.663227	-0.099954
H	2.263067	0.035497	-1.262948
H	2.785566	0.542708	0.361547
C	1.645620	-4.885967	-1.289723
H	0.604665	-5.099145	-1.602094
H	2.067185	-5.827001	-0.894159
H	2.209664	-4.612904	-2.199298
C	1.637046	-3.490790	3.553694
H	2.266708	-2.835874	4.179235
H	2.032230	-4.517965	3.638050
H	0.632974	-3.483941	4.013829
C	0.709161	-0.726753	4.915584
C	1.450160	-0.458735	6.101790
C	0.898203	-0.794022	7.354652
H	1.475320	-0.576552	8.264672
C	-0.368400	-1.394240	7.475048
C	-1.074348	-1.667695	6.291622
H	-2.062702	-2.144848	6.359085
C	-0.565584	-1.347970	5.014168
C	2.820070	0.194474	6.080429
H	3.533561	-0.352465	5.436854
H	3.252497	0.235493	7.095036
H	2.775070	1.232747	5.698490
C	-0.930377	-1.766566	8.828759
H	-2.034376	-1.785318	8.819984
H	-0.605317	-1.058891	9.612004
H	-0.586694	-2.773772	9.135103
C	-1.430143	-1.683905	3.818314
H	-2.086808	-2.543479	4.040331
H	-0.835795	-1.930483	2.923219
H	-2.077391	-0.830418	3.543820
N	-0.983919	3.067401	5.303822
Sb	1.577997	0.035324	3.042116

Table S14 Cartesian coordinates (Å) of the optimized structure of [2-(Me_2NHCH_2)C_6H_5]$^+$; cation of **3**.

Atom	x	y	z
H	0.915061	1.126705	3.787861
C	-0.411035	0.349981	1.682162
C	-0.887759	1.680880	1.671581
H	-0.193301	2.519294	1.827989
C	-2.244291	1.943889	1.425394
H	-2.607193	2.978222	1.410471
C	-3.130758	0.880050	1.176448
H	-4.188418	1.086312	0.974024
C	-2.661209	-0.445581	1.171405

H	4.929482	3.962372	1.091483
C	5.977066	5.963104	5.211790
H	6.896259	6.115273	5.823339
H	5.448290	6.936071	5.169347
C	4.411404	5.533561	7.045954
H	5.146631	5.706307	7.863128
H	3.638019	4.820542	7.382944
H	3.915739	6.487215	6.800601
C	5.761836	3.725485	6.159001
H	6.576975	3.899819	6.895979
H	6.178961	3.279936	5.241066
H	5.032406	3.004835	6.567173
C	2.812288	6.540825	4.213319
C	3.397456	7.580935	3.462683
H	4.144632	7.348090	2.691551
C	3.026974	8.917495	3.696143
H	3.490435	9.722735	3.110448
C	2.060720	9.220051	4.673224
H	1.770544	10.263467	4.854978
C	1.462930	8.182253	5.409972
H	0.702173	8.411786	6.167783
C	1.834292	6.843246	5.183134
H	1.377421	6.029240	5.764257
Cl	2.306549	4.490903	1.654024
Cl	1.351401	3.552137	6.542526
Cl	4.410913	1.452080	3.663078
Cl	2.630441	0.439350	6.379086
N	5.068602	4.993024	5.845725
Pd	2.829579	2.395488	5.125657
Sb	3.414248	4.492332	3.862632

Table S15 Cartesian coordinates (Å) of the optimized structure of [{2-(Me_2NCH_2)C_6H_4}$Mes_2SbPdCl_2$] (**4**); N coordinated to Pd.

Atom	x	y	z
C	-0.283228	2.165712	2.164917
C	-1.093621	2.270876	3.320383
C	-2.297347	1.535367	3.374846
H	-2.928377	1.607518	4.271015
C	-2.697533	0.721211	2.303441
H	-3.637607	0.159427	2.364400
C	-1.891957	0.632299	1.154899
H	-2.197358	-0.001025	0.312602
C	-0.689298	1.355624	1.088088
H	-0.059120	1.281776	0.191026
C	-0.688997	3.128329	4.502079
H	-1.296592	2.826146	5.380473
H	0.369648	2.955365	4.772617
C	-2.264996	4.919470	3.926505
H	-2.974931	4.498524	4.669316
H	-2.466588	4.472383	2.940924
H	-2.382236	6.012370	3.860235
C	-0.567986	5.249087	5.647663
H	-0.673090	6.341144	5.553747
H	0.467135	5.008910	5.941295
H	-1.264619	4.860202	6.419574
C	2.133390	3.138866	0.078638
C	1.222652	3.528457	-0.944527
C	1.572892	3.265383	-2.284547
H	0.871336	3.560678	-3.076942
C	2.796786	2.670275	-2.638358
H	-3.349884	-1.272604	0.962734
C	-1.306247	-0.711733	1.427012
H	-0.940239	-1.747040	1.413497
C	1.032717	0.082741	2.001567
H	1.357381	-0.933364	1.719985
H	1.706717	0.813688	1.521957
C	0.557192	-0.829021	4.316823
H	-0.513413	-0.767018	4.070895
H	0.715402	-0.638656	5.389225
H	0.949615	-1.821839	4.047361
C	2.772774	0.208091	3.830044
H	2.916401	0.341655	4.913224
H	3.259602	1.029078	3.281735
H	3.197362	-0.756903	3.512933
N	1.301064	0.207959	3.518480

Table S16 Cartesian coordinates (Å) of the optimized structure of [{2-(Me_2NCH_2)C_6H_4}$Mes_2SbPdCl_2$]; N coordinated to Sb.

Atom	x	y	z
C	-0.447640	2.522179	1.499861
C	-1.207285	2.298401	2.673942
C	-2.295572	1.402473	2.616469
H	-2.892206	1.240672	3.524350
C	-2.621154	0.717395	1.436569
H	-3.473912	0.027612	1.419367
C	-1.845625	0.920101	0.284842
H	-2.072623	0.382120	-0.643726
C	-0.766107	1.817656	0.321574
H	-0.146824	1.924511	-0.575329
C	-0.848674	2.910222	4.013189
H	-1.698630	2.762864	4.721907
H	0.016373	2.362875	4.437974
C	-1.621401	5.139366	3.477336
H	-2.466101	5.075680	4.201973
H	-1.972361	4.805915	2.488217
H	-1.308017	6.189235	3.372687
C	0.020508	4.813074	5.205480
H	0.365810	5.854637	5.099682
H	0.863884	4.189133	5.543411
H	-0.771254	4.785499	5.989875
C	2.308728	3.089481	-0.295392
C	1.622139	3.349236	-1.515856
C	2.175741	2.862103	-2.718341
H	1.636196	3.050647	-3.657230
C	3.403833	2.180427	-2.757371

C	3.705360	2.374113	-1.606440	C	4.109521	2.041326	-1.549565
H	4.690625	1.961446	-1.864874	H	5.105533	1.576842	-1.564056
C	3.410090	2.607370	-0.247204	C	3.603200	2.498890	-0.315162
C	-0.055374	4.289581	-0.665544	C	0.390455	4.225475	-1.624926
H	-0.646228	4.419384	-1.587592	H	-0.217472	3.950981	-2.504542
H	0.184746	5.294568	-0.267358	H	0.696477	5.282495	-1.743534
H	-0.708861	3.792352	0.072862	H	-0.276188	4.211315	-0.747967
C	3.129777	2.363720	-4.080646	C	3.951651	1.630795	-4.054558
H	2.844821	1.324384	-4.335625	H	3.543242	0.621147	-4.255306
H	4.211684	2.463194	-4.278373	H	5.051658	1.540871	-4.027490
H	2.590521	3.031867	-4.774513	H	3.679828	2.269238	-4.913802
C	4.490943	2.324552	0.776040	C	4.502322	2.389538	0.898135
H	4.593279	3.145495	1.506527	H	4.476275	3.314394	1.499908
H	5.467129	2.201115	0.277544	H	5.546873	2.231967	0.580374
H	4.297666	1.404932	1.356080	H	4.229279	1.550686	1.561797
C	2.767482	2.406923	3.490985	C	2.348388	2.782986	3.211076
C	3.515047	3.200036	4.405111	C	2.938632	3.545980	4.253576
C	4.272923	2.541540	5.396100	C	3.445409	2.861409	5.380869
H	4.852571	3.150199	6.103941	H	3.895680	3.453820	6.189484
C	4.321571	1.139791	5.499432	C	3.398638	1.463438	5.501449
C	3.594256	0.385083	4.561050	C	2.838459	0.736274	4.436141
H	3.638377	-0.712356	4.607398	H	2.809655	-0.361077	4.493896
C	2.817614	0.987990	3.550604	C	2.316295	1.359970	3.284699
C	3.554607	4.711878	4.349122	C	3.100102	5.046037	4.222267
H	3.822502	5.094256	3.346224	H	4.012079	5.327049	3.665210
H	4.285523	5.115766	5.069223	H	3.177799	5.456186	5.243329
H	2.569065	5.165363	4.576108	H	2.271622	5.556713	3.704000
C	5.169885	0.461947	6.551571	C	3.969308	0.756311	6.709581
H	4.704183	-0.473780	6.908417	H	3.342457	-0.102038	7.010741
H	5.338900	1.117144	7.423665	H	4.061871	1.435424	7.574579
H	6.163555	0.196460	6.141514	H	4.979457	0.360322	6.489656
C	2.099981	0.087243	2.566982	C	1.768980	0.451116	2.199984
H	2.597248	-0.896025	2.505555	H	2.306377	-0.512889	2.208727
H	2.074993	0.512070	1.547408	H	1.871621	0.873065	1.186235
H	1.050030	-0.086537	2.865531	H	0.695901	0.234973	2.353248
Cl	2.052652	6.538398	1.434102	N	-0.481209	4.325171	3.917351
Cl	-0.439949	7.701568	3.406900	Sb	1.349088	3.738776	1.546796
N	-0.862693	4.619555	4.326870	Cl	-0.743442	6.721126	0.731049
Pd	0.503109	5.603831	2.881890	Cl	3.724947	6.053371	1.085425
Sb	1.463767	3.426548	2.096534	Pd	1.431408	6.184809	1.132062

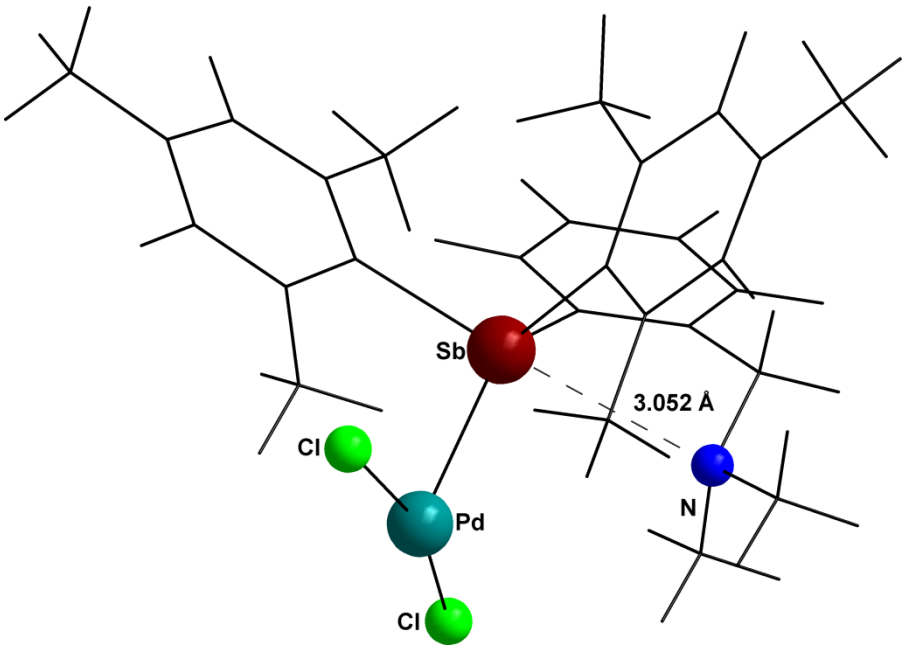

Fig. S14 Theoretically calculated alternative structure for compound **4**. Nitrogen atom is weakly coordinated to antimony (N···Sb 3.052 Å).