ESI for:

Antimony centre in three different roles: Donor strength or acceptor ability determines the bonding pattern?

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1) General procedures.

All manipulations were carried out under an argon atmosphere using standard Schlenk tube technique. Solvents were dried using Pure Solv–Innovative Technology equipment. C_6D_6, CD_2Cl_2 and $CDCl_3$ were dried by standard procedures and stored over potassium mirror (benzene) or molecular sieves, respectively. Precursors of the ligand ArBr was synthesized according to literature.[17] All reagents other reagents were purchased from commercial sources and used as delivered**.** ^1H and $^{13}C\{^1H\}$ NMR spectra were recorded on Bruker Ascend 500 MHz and Bruker Ultrashield 400 MHz spectrometers, using a 5 mm tunable broad-band probe or a cryo-probe Prodigy. Appropriate chemical shifts in ^1H and $^{13}C\{^1H\}$ NMR spectra are given relative to the residual signals of the solvent [C_6D_6: $\delta(^1H) = 7.16$ ppm and $\delta(^{13}C) = 138.9$ ppm, CD_2Cl_2: $\delta(^1H) = 5.32$ ppm and $\delta(^{13}C) = 54.00$ ppm, $CDCl_3$: $\delta(^1H) = 7.27$ ppm and $\delta(^{13}C) = 77.23$ ppm.] Elemental analyses were performed on an LECO-CHNS-932 analyser.

2) Syntheses.

Preparation of [2-(Me$_2$N)$_2$C=NC$_6$H$_4$]SbCl$_2$ - ArSbCl$_2$.

A sample 415 mg of ArLi[S1] (2.1 mmol) dissolved in toluene (20 mL) was added to a solution of $SbCl_3$ 480 mg (2.1 mmol) in toluene (20 mL) at 0 °C. The temperature was kept at this temperature for 30 min and then gradually warmed to r.t. and stirred overnight. The resulting mixture was filtered and the filtrate was concentrated and stored at -30°C. Colorless crystals of **ArSbCl$_2$** were obtained in a period of several days that were collected by filtration and dried *in vacuo*. Single-crystals suitable for X-ray diffraction analysis could be obtained by re-crystallization from saturated dichloromethane solution layered with hexane. Yield: 393 mg, (49 %), m. p. 143°C. Anal. Calcd for $C_{11}H_{16}Cl_2N_3Sb$ (MW 382.93): C 34.5; H 4.2; N 11.0 % Found: C, 34.6; H, 4.4; N 11.2%. **^{1}H NMR** (500 MHz, C_6D_6) δ (ppm): 2.21 [12H, s(br), CH_3]; 6.29 [1H, d, ^3J(^{1}H,^{1}H) = 7.8 Hz, Ar-*H*]; 7.02 [1H, t, ^3J(^{1}H,^{1}H) = 7.3 Hz, Ar-*H*]; 7.22 [1H, t, ^3J(^{1}H,^{1}H) = 7.3 Hz, Ar-*H*]; 8.35 [1H, d, ^3J(^{1}H,^{1}H) = 7.3 Hz, Ar-*H*]. **^{13}C{^{1}H} NMR** (125.76 MHz, C_6D_6) δ (ppm): 39.5 [*C*H$_3$]; 118.4 [Ar-*C*H]; 123.1 [Ar-*C*H]; 132.1 [Ar-*C*H]; 132.7 [Ar-*C*H]; 146.8 [Ar-*C*]; 155.2 [Ar-*C*]; 159.2 [*C*=N].

Preparation of {[2-(Me$_2$N)$_2$C=NC$_6$H$_4$]}$_2$SbCl – Ar$_2$SbCl.

A sample 1.874 g of ArLi[S1] (9.5 mmol) dissolved in toluene (20 mL) was added to a solution of $SbCl_3$ 1.084 g (4.75 mmol) in toluene (20 mL) at 0 °C. The temperature was kept at this temperature for 30 min and then gradually warmed to r.t. and stirred overnight. The resulting mixture was filtered and the filtrate was concentrated to *ca*. 5 mL and layered by hexane. Storage of this mixture resulted in the formation of colorless crystals of **Ar$_2$SbCl** within 24 h. These crystals were collected by filtration and dried *in vacuo*. Single-crystals suitable for X-ray diffraction analysis could be obtained by re-crystallization from saturated benzene solution layered with hexane. Yield: 1.47 g, (58 %), m. p. 173°C. Anal. Calcd for $C_{22}H_{32}ClN_6Sb$ (MW 537.75): C 49.1; H 6.0; N 15.6 % Found: C, 49.5; H, 6.3; N 15.2%. **^{1}H NMR** (500 MHz, C_6D_6)

δ (ppm): 2.33 [12H, s(br), CH_3]; 6.46 [1H, d, $^3J(^1H,^1H)$ = 7.8 Hz, Ar-*H*]; 6.96 [1H, t, $^3J(^1H,^1H)$ = 7.5 Hz, Ar-*H*]; 7.22 [1H, t, $^3J(^1H,^1H)$ = 7.6 Hz, Ar-*H*]; 8.19 [1H, d, $^3J(^1H,^1H)$ = 7.4 Hz, Ar-*H*]. **$^{13}C\{^1H\}$ NMR** (125.76 MHz, C_6D_6) δ (ppm): 39.7 [*C*H_3]; 118.9 [Ar-*C*H]; 122.4 [Ar-*C*H]; 129.9 [Ar-*C*H]; 135.3 [Ar-*C*H]; 142.2 [Ar-*C*]; 155.3 [Ar-*C*]; 158.9 [*C*=N].

Preparation of {[2-$(Me_2N)_2C$=NC_6H_4]}$_3$Sb – Ar_3Sb.

A sample 1.20 g of ArLi[S1] (6.09 mmol) dissolved in toluene (20 mL) was added to a solution of $SbCl_3$ 421 mg (1.85 mmol) in toluene (20 mL) at 0 °C. The temperature was kept at this temperature for 30 min and then gradually warmed to r.t. and stirred for 6 days. The resulting mixture was filtered and the filtrate was evaporated. The resulting solid was washed with hexane (15 mL) and dried *in vacuo* to give **Ar_3Sb** as white powder. Single-crystals suitable for X-ray diffraction analysis could be obtained by crystallization from saturated hexane solution at -30°C. Yield: 858 mg, (67 %), m. p. 148°C. Anal. Calcd for $C_{33}H_{48}N_9Sb$ (MW 692.57): C 57.2; H 7.0; N 18.2 % Found: C, 57.6; H, 7.3; N 18.3%. **^1H NMR** (500 MHz, C_6D_6) δ (ppm): 2.42 [12H, s, CH_3]; 6.67 [1H, d, $^3J(^1H,^1H)$ = 7.8 Hz, Ar-*H*]; 6.86 [1H, t, $^3J(^1H,^1H)$ = 7.3 Hz, Ar-*H*]; 7.24 [1H, t, $^3J(^1H,^1H)$ = 7.2 Hz, Ar-*H*]; 7.77 [1H, d, $^3J(^1H,^1H)$ = 7.4 Hz, Ar-*H*]. **$^{13}C\{^1H\}$ NMR** (125.76 MHz, C_6D_6) δ (ppm): 40.0 [*C*H_3]; 119.8 [Ar-*C*H]; 121.3 [Ar-*C*H]; 128.8 [Ar-*C*H]; 136.4 [Ar-*C*]; 138.4 [Ar-*C*H]; 156.9 [Ar-*C*]; 157.6 [*C*=N].

Preparation of [$Ar_3SbPdCl_2$] – complex 1.

A sample 218 mg of **Ar_3Sb** (0.31 mmol) and 82 mg of *cis*-[$PdCl_2(CH_3CN)_2$] (0.31 mmol) was dissolved in dichloromethane (10 mL) and stirred for 1 h. The resulting mixture was filtered and the filtrate was concentrated and layered with hexane. Storage of this mixture at -30°C provided orange-brown single-crystals of **1** that were collected by decantation, washed with hexane and dried *in vacuo*. Yield: 226 mg, (82 %), m. p. 149°C. Anal. Calcd for $C_{33}H_{48}Cl_2N_9PdSb$ (MW 869.89): C 45.6; H 5.6; N 14.5 % Found: C, 45.9; H, 5.7; N 14.2%. **^1H NMR** (500 MHz, $CDCl_3$) δ (ppm): 2.61 [24H, s, CH_3]; 3.03 [12H, s, CH_3]; 6.22 [1H, d,

$^3J(^1H,^1H)$ = 8.1 Hz, Ar-*H*]; 6.47 [2H, d, $^3J(^1H,^1H)$ = 8.1 Hz, Ar-*H*]; 6.64 [1H, t, $^3J(^1H,^1H)$ = 7.5 Hz, Ar-*H*]; 6.74 [2H, t, $^3J(^1H,^1H)$ = 7.5 Hz, Ar-*H*]; 7.12 [1H, m, Ar-*H*]; 7.25 [2H, m, Ar-*H*]; 7.36 [2H, d(br), Ar-*H*]; 7.70 [1H, d(br), Ar-*H*]. **$^{13}C\{^1H\}$ NMR** (125.76 MHz, $CDCl_3$) δ (ppm): 40.0 [*C*H_3]; 40.4 [*C*H_3]; 41.7 [*C*H_3];114.6 [Ar-*C*H]; 118.8 [Ar-*C*H]; 118.9 [Ar-*C*H]; 120.0 [Ar-*C*H]; 128.5 [Ar-*C*]; 129.1 [Ar-*C*]; 130.5 [Ar-*C*H]; 130.9 [Ar-*C*H]; 135.3 [Ar-*C*H]; 136.9 [Ar-*C*H]; 153.6 [Ar-*C*]; 155.1 [Ar-*C*]; 159.4 [*C*=N]; 168.9 [*C*=N].

Preparation of [$Ar_3SbPtCl_2$] – complex 2.

A sample 160 mg of **Ar_3Sb** (0.23 mmol) and 61mg of $PtCl_2$ (0.23 mmol) was suspended in dichloromethane (10 mL) and stirred for 3 h and during this period $PtCl_2$ dissolved. The resulting mixture was filtered and the filtrate was concentrated and layered with hexane. Storage of this mixture at -30°C provided orange single-crystals of **2** that were collected by decantation, washed with hexane and dried *in vacuo*. Yield: 158 mg, (72 %), m. p. 140°C. Anal. Calcd for $C_{33}H_{48}Cl_2N_9PtSb$ (MW 985.55): C 41.4; H 5.1; N 13.2 % Found: C, 41.6; H, 5.5; N 13.5%. **^1H NMR** (500 MHz, CD_2Cl_2) δ (ppm): 2.54 [24H, s, C*H*$_3$]; 2.88 [12H, s, C*H*$_3$]; 3.07 [12H, s, C*H*$_3$]; 6.20 [1H, d, $^3J(^1H,^1H)$ = 8.4 Hz, Ar-*H*]; 6.40 [2H, d, $^3J(^1H,^1H)$ = 8.0 Hz, Ar-*H*]; 6.63 [1H, t, $^3J(^1H,^1H)$ = 7.1 Hz, Ar-*H*]; 6.75 [2H, t, $^3J(^1H,^1H)$ = 7.1 Hz, Ar-*H*]; 7.07 [1H, t, $^3J(^1H,^1H)$ = 7.5 Hz, Ar-*H*]; 7.20 [2H, t, $^3J(^1H,^1H)$ = 7.5 Hz, Ar-*H*]; 7.45 [2H, d, $^3J(^1H,^1H)$ = 6.4 Hz, Ar-*H*]; 8.22 [1H, d $^3J(^1H,^1H)$ = 5.5 Hz, Ar-*H*]. **$^{13}C\{^1H\}$ NMR** (125.76 MHz, CD_2Cl_2) δ (ppm): 40.0 [*C*H_3]; 40.1 [*C*H_3]; 42.0 [*C*H_3];113.9 [Ar-*C*H]; 119.2 [Ar-*C*H]; 119.6 [Ar-*C*H]; 120.1 [Ar-*C*H]; 126.3 [Ar-*C*]; 127.4 [Ar-*C*]; 131.0 [Ar-*C*H]; 131.2 [Ar-*C*H]; 135.3 [Ar-*C*H]; 138.4 [Ar-*C*H]; 155.5 [Ar-*C*]; 155.8 [Ar-*C*]; 159.9 [*C*=N]; 169.6 [*C*=N].

Preparation of [$Ar_2SbClPdCl_2$] – complex 3.

A sample 136 mg of **Ar_2SbCl** (0.25 mmol) and 66 mg of *cis*-[$PdCl_2(CH_3CN)_2$] (0.25 mmol) was dissolved in acetonitrile (15 mL) and stirred for 1 h. During this period, a red precipitate formed that was isolated by filtration and dried *in vacuo* to give **3**. Single-crystals suitable for

X-ray diffraction analysis could be obtained by storing the mother liquor for several hours at r.t.. Yield: 149 mg, (83 %), m. p. 188°C. Anal. Calcd for $C_{22}H_{32}Cl_3N_6PdSb$ (MW 715.07): C 37.0; H 4.5; N 11.8 % Found: C, 37.2; H, 4.1; N 11.4%. **^{1}H NMR** (500 MHz, CD_2Cl_2) δ (ppm): 0.83 [3H, s, C*H*$_3$]; 2.20 [3H, s, C*H*$_3$]; 2.48 [3H, s, C*H*$_3$]; 2.61 [3H, s, C*H*$_3$]; 2.86 [3H, s, C*H*$_3$]; 2.96 [3H, s, C*H*$_3$]; 3.74 [3H, s, C*H*$_3$]; 3.75 [3H, s, C*H*$_3$]; 6.15 [1H, d, ^3J(^{1}H,^{1}H) = 7.5 Hz, Ar-*H*]; 6.26 [1H, d, ^3J(^{1}H,^{1}H) = 7.8 Hz, Ar-*H*]; 7.00 [1H, t, ^3J(^{1}H,^{1}H) = 7.2 Hz, Ar-*H*]; 7.08 [3H, m, Ar-*H*]; 8.12 [1H, d, ^3J(^{1}H,^{1}H) = 7.1 Hz, Ar-*H*]; 8.17 [2H, d, ^3J(^{1}H,^{1}H) = 7.3 Hz, Ar-*H*]. **^{13}C{^{1}H} NMR** (125.76 MHz, CD_2Cl_2) δ (ppm): 37.5 [*C*H$_3$]; 39.6 [*C*H$_3$]; 39.9 [*C*H$_3$]; 40.5 [*C*H$_3$]; 42.1 [*C*H$_3$]; 42.5 [*C*H$_3$]; 42.8 [*C*H$_3$]; 123.9 [Ar-*C*H]; 123.9 [Ar-*C*H]; 124.2 [Ar-*C*H]; 124.8 [Ar-*C*H]; 129.2 [Ar-*C*H]; 130.3 [Ar-*C*H]; 135.3 [Ar-*C*H]; 135.5 [Ar-*C*H]; 138.4 [Ar-*C*]; 139.4 [Ar-*C*]; 154.9 [Ar-*C*]; 155.9 [Ar-*C*]; 165.9 [*C*=N]; 169.9 [*C*=N].

Preparation of [$Ar_2SbClPtCl_2$] – complex 4.

A sample 136 mg of **Ar_2SbCl** (0.25 mmol) and 67 mg of $PtCl_2$ (0.25 mmol) was dissolved in chloroform (15 mL) and heated to 60 °C for 1h giving orange solution. The mixture was filtered when still hot and slow cooling of the filtrate provided yellow single-crystals of **4** that was isolated by filtration and dried *in vacuo* Yield: 84 mg, (42 %), m. p. 230°C. Anal. Calcd for $C_{22}H_{32}Cl_3N_6PtSb$ (MW 803.73): C 32.9; H 4.0; N 10.5 % Found: C, 33.2; H, 4.2; N 10.2%.

3) NMR spectra of studied compounds.

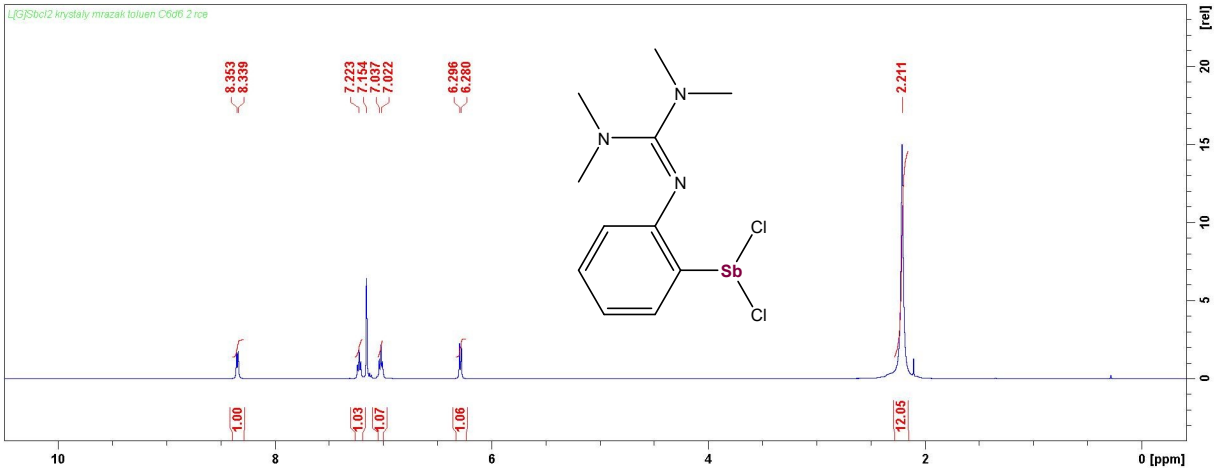


Figure S1: ^{1}H NMR spectrum of **$ArSbCl_2$** in C_6D_6 (500 MHz).

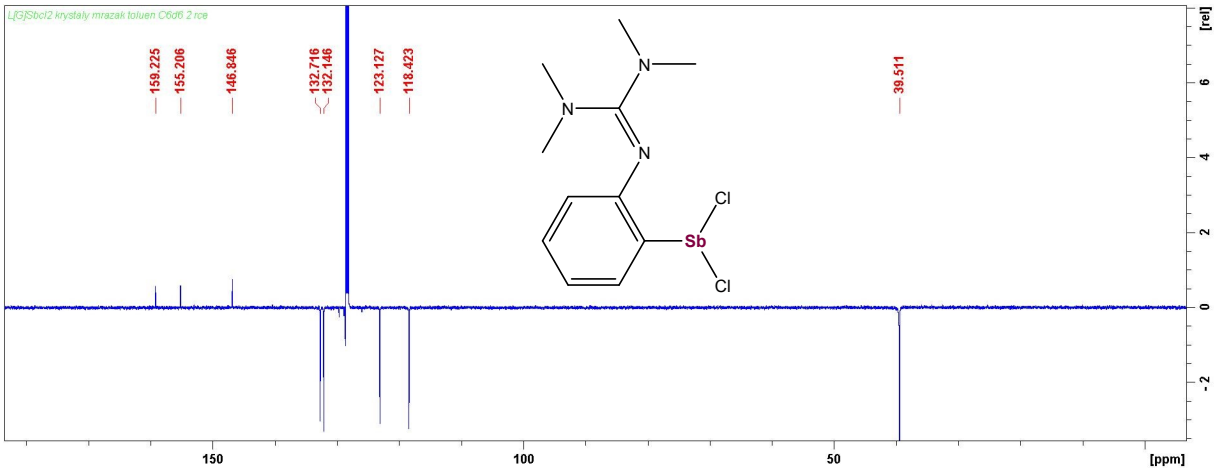


Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum of **$ArSbCl_2$** in C_6D_6 (125.6 MHz).

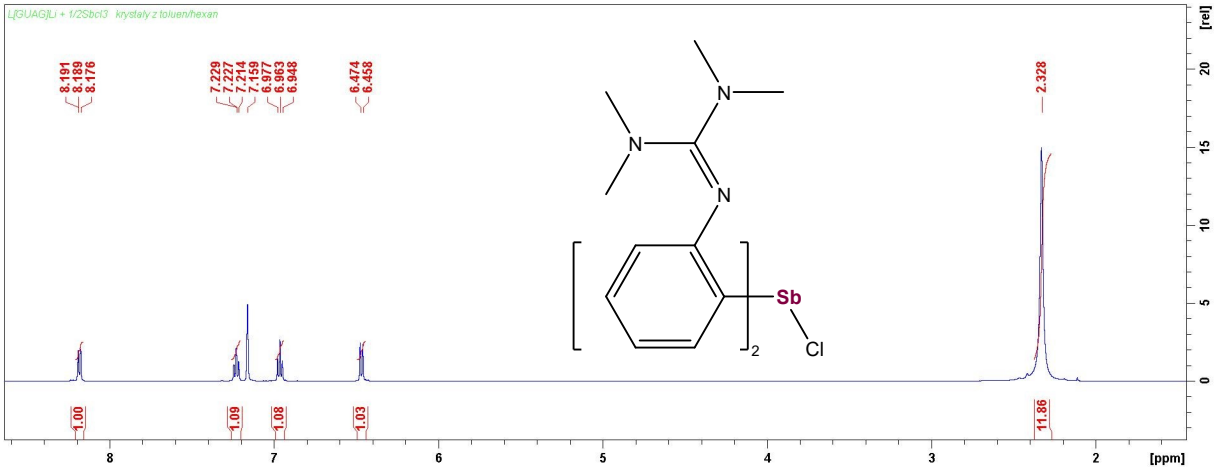


Figure S3: ^{1}H NMR spectrum of **Ar_2SbCl** in C_6D_6 (500 MHz).

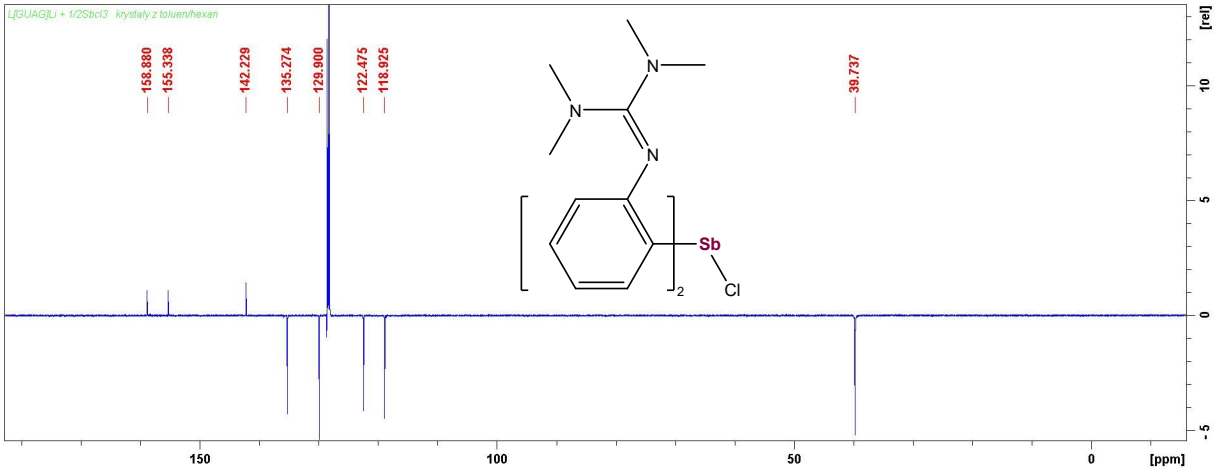


Figure S4: $^{13}C\{^{1}H\}$ NMR spectrum of **Ar_2SbCl** in C_6D_6 (125.6 MHz).

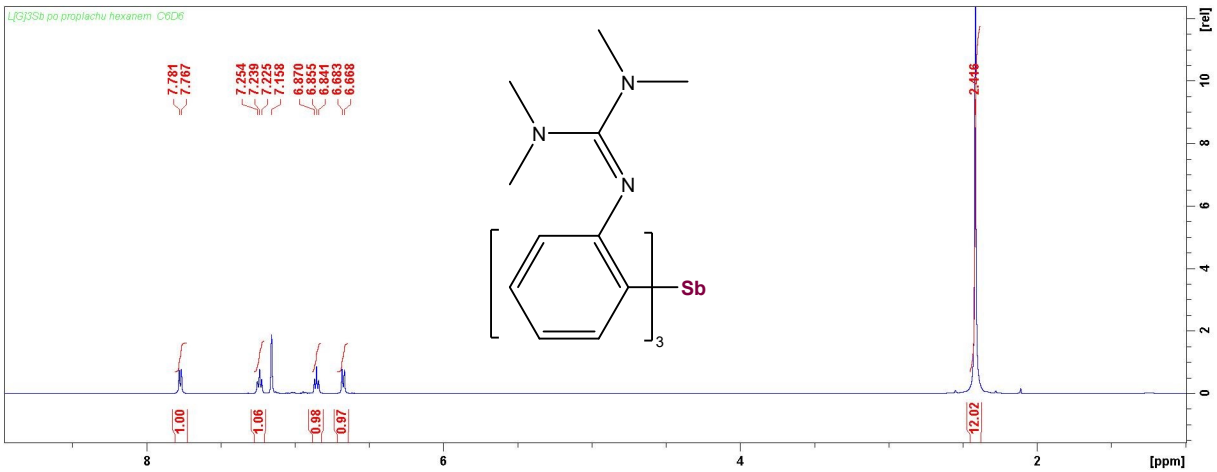


Figure S5: ^{1}H NMR spectrum of **Ar_3Sb** in C_6D_6 (500 MHz).

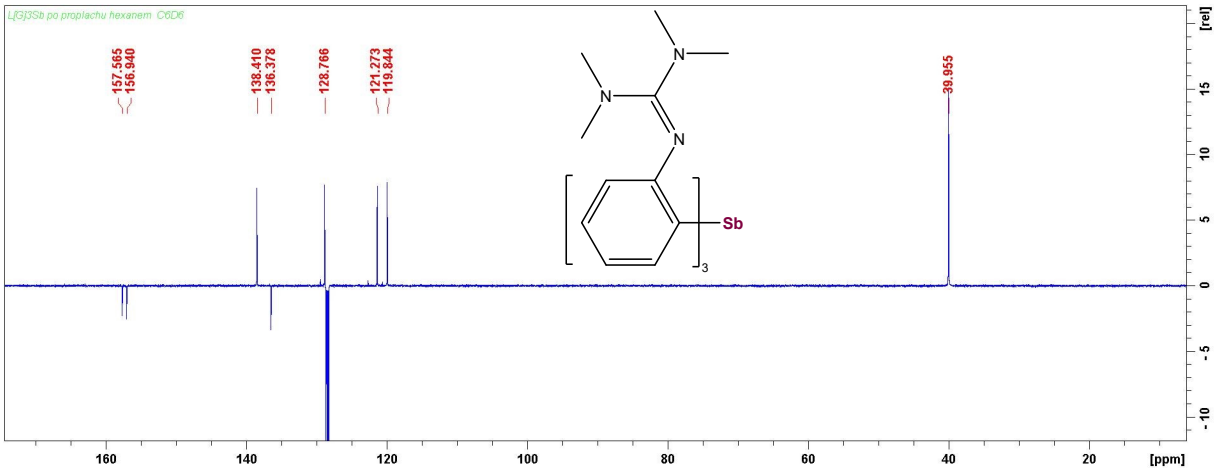


Figure S6: $^{13}C\{^{1}H\}$ NMR spectrum of **Ar_3Sb** in C_6D_6 (125.6 MHz).

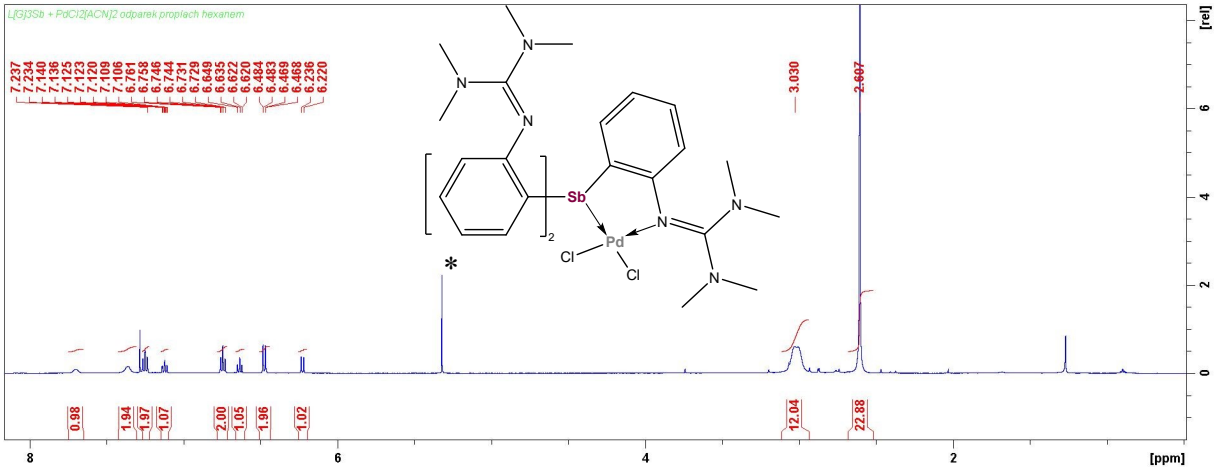


Figure S7: ^{1}H NMR spectrum of complex **1** in $CDCl_3$ (500 MHz). *denotes residual signal of co-crystallized dichloromethane.

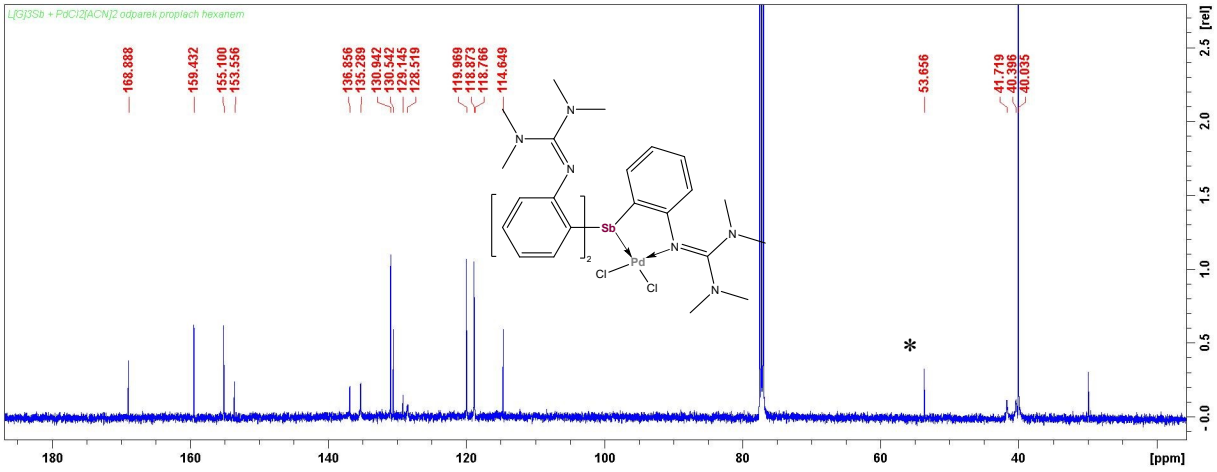


Figure S8: $^{13}C\{^{1}H\}$ NMR spectrum of complex **1** in $CDCl_3$ (125.6 MHz). *denotes residual signal of co-crystallized dichloromethane.

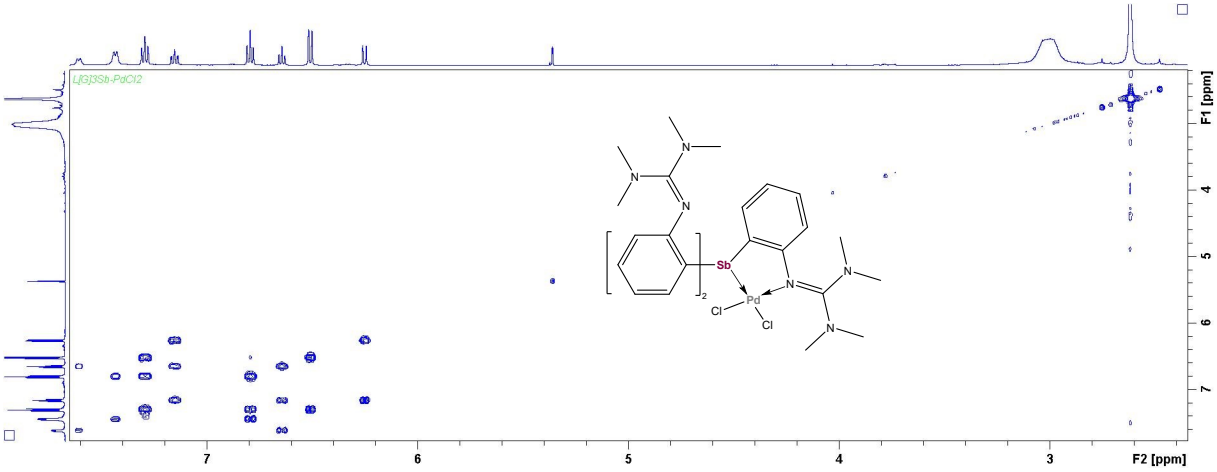


Figure S9: ^{1}H-^{1}H COSY NMR spectrum of complex **1** in CD_2Cl_2 (500 MHz).

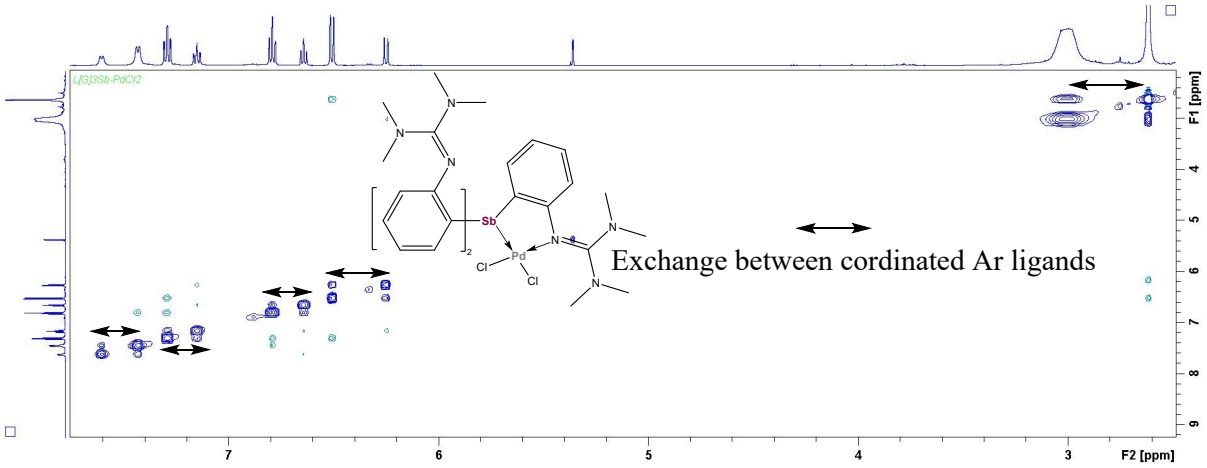


Figure S10: ^{1}H-^{1}H EXSY NMR spectrum of complex **1** in CD_2Cl_2 (mixing time 1s, 500 MHz).

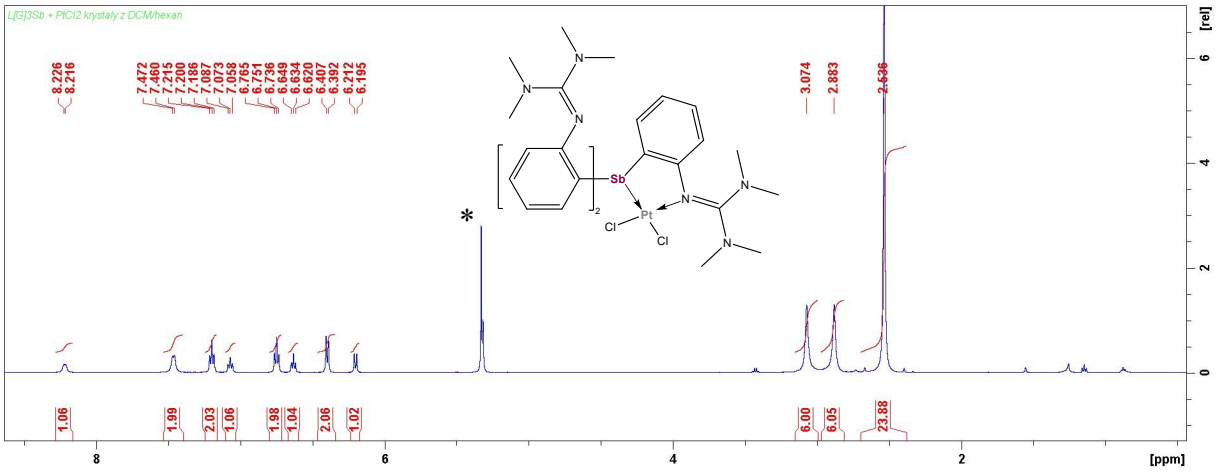


Figure S11: ^{1}H NMR spectrum of complex **2** in CD_2Cl_2 (500 MHz). *denotes residual signal of co-crystallized dichloromethane.

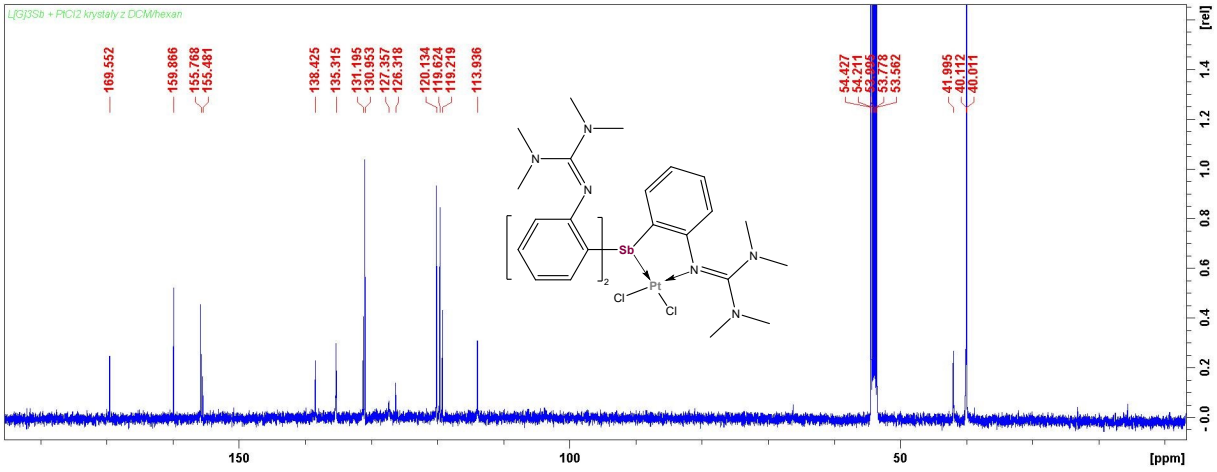


Figure S12: $^{13}C\{^{1}H\}$ NMR spectrum of complex **2** in CD_2Cl_2 (125.6 MHz).

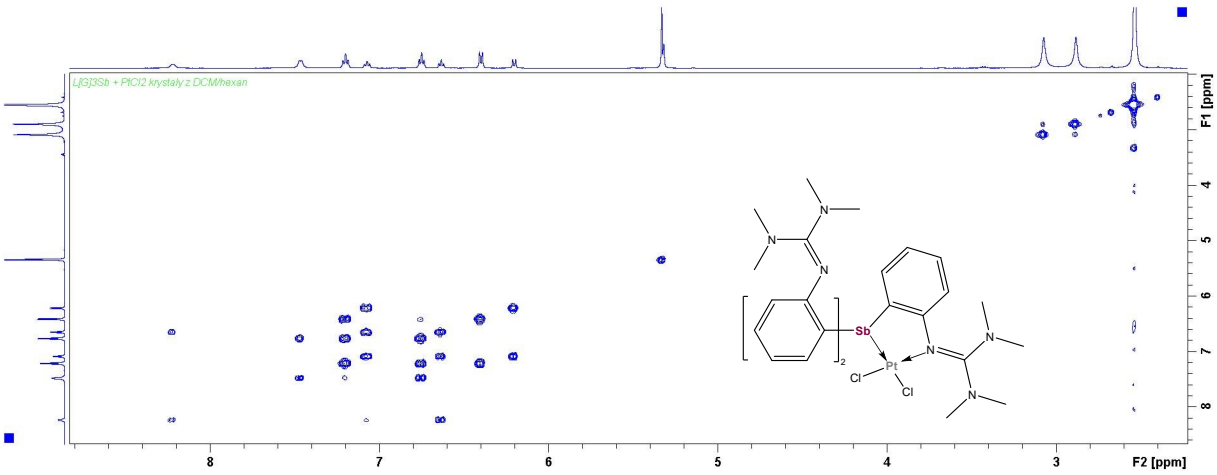


Figure S13: ^{1}H-^{1}H COSY NMR spectrum of complex **2** in CD_2Cl_2 (500 MHz).

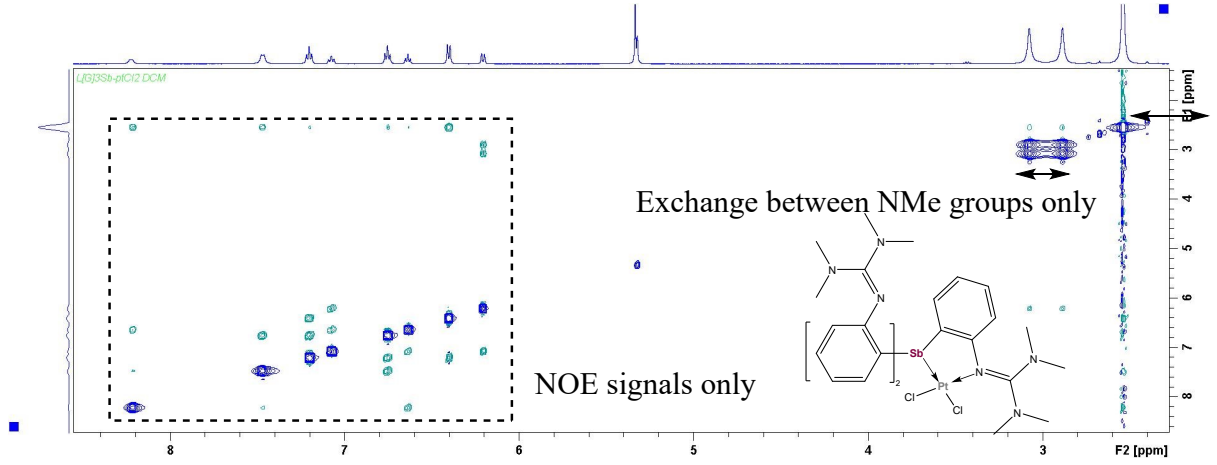


Figure S14: ^{1}H-^{1}H EXSY NMR spectrum of complex **2** in CD_2Cl_2 (mixing time 1s, 500 MHz).

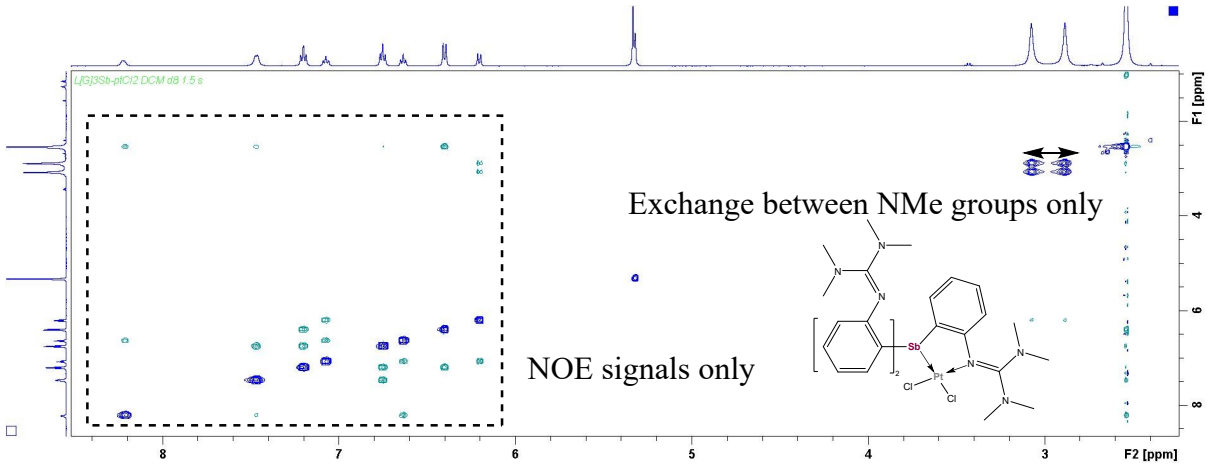


Figure S15: ^{1}H-^{1}H EXSY NMR spectrum of complex **2** in CD_2Cl_2 (mixing time 1.5s, 500 MHz).

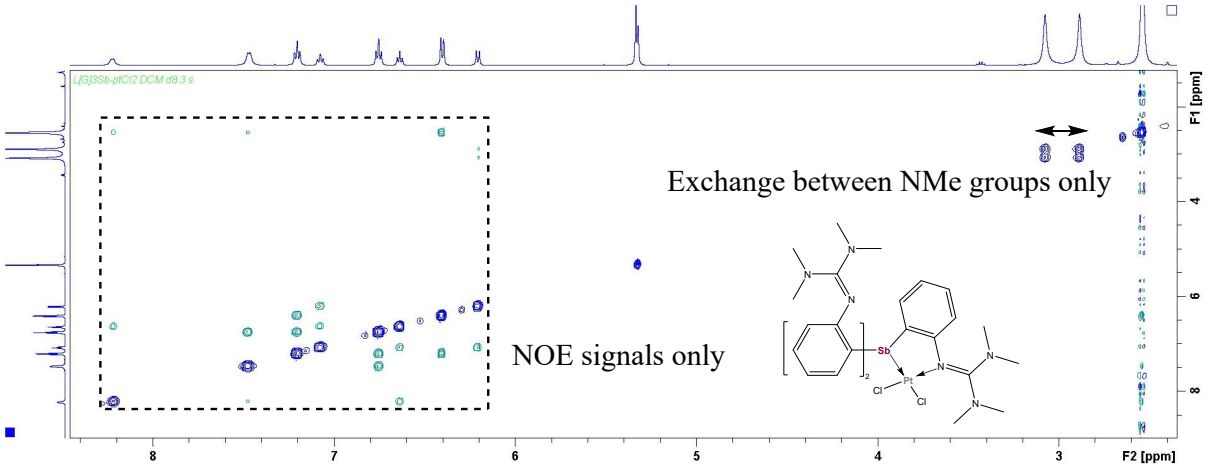


Figure S16: ^{1}H-^{1}H EXSY NMR spectrum of complex **2** in CD_2Cl_2 (mixing time 3s, 500 MHz).

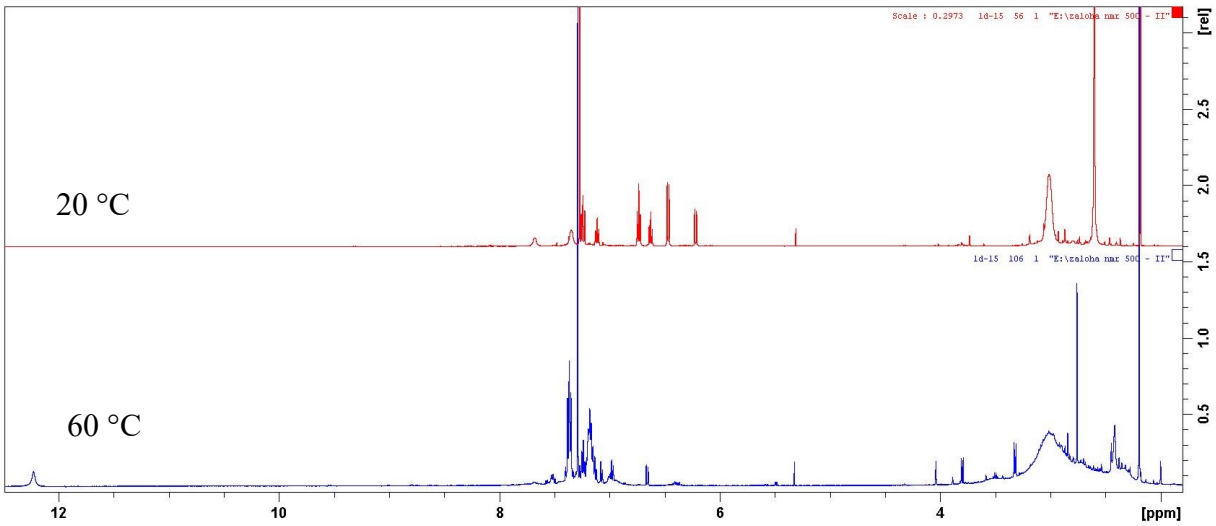


Figure S17: ^{1}H NMR spectra showing decomposition (irreversible changes in spectra) of the complex **1** in $CDCl_3$ upon heating (500 MHz).

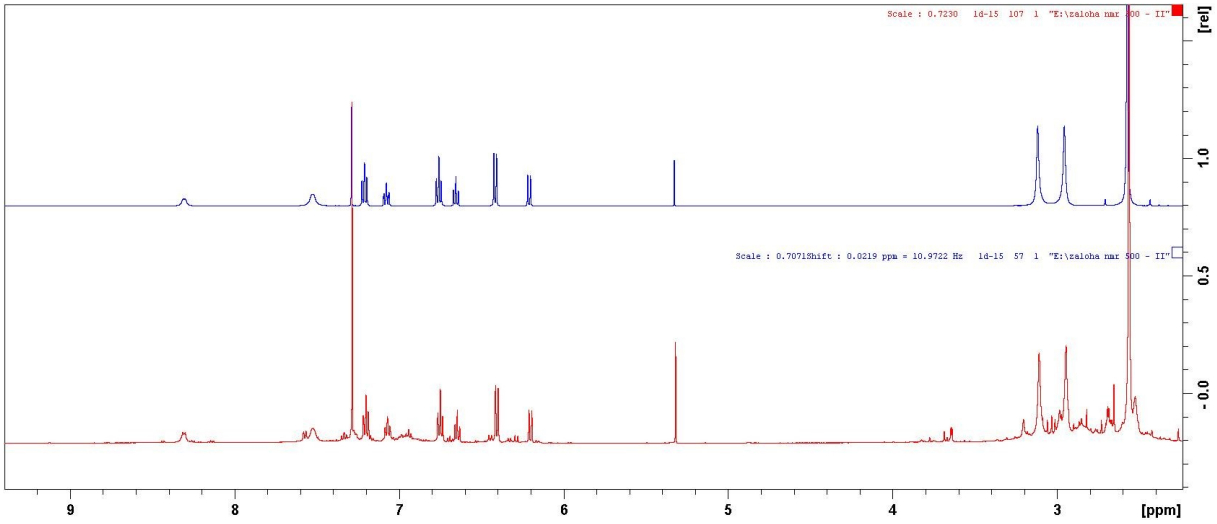


Figure S18: ^{1}H NMR spectra showing decomposition (irreversible changes in spectra) of the complex **2** in $CDCl_3$ upon heating (500 MHz).

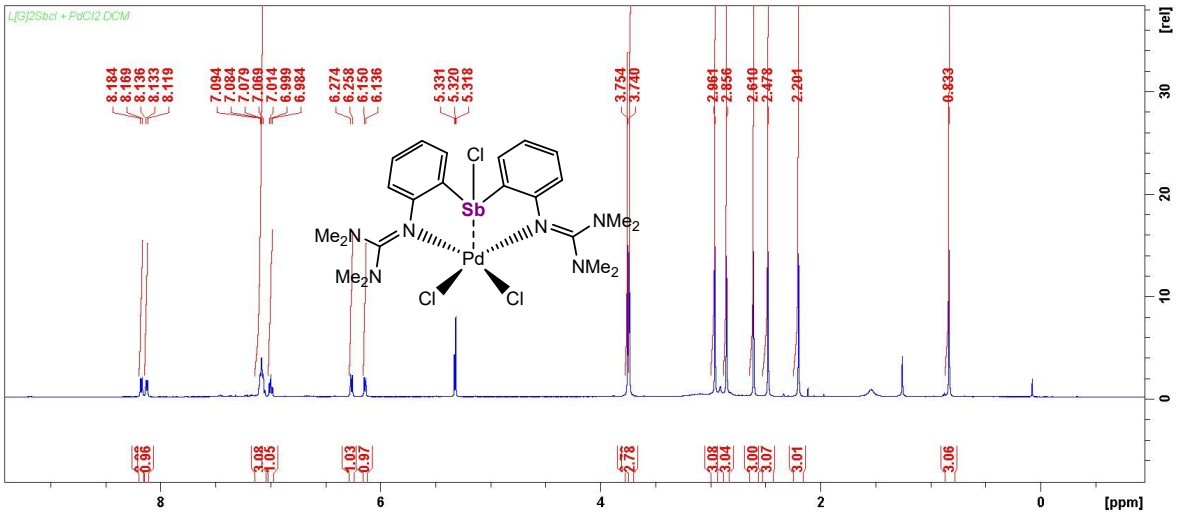


Figure S19: ^{1}H NMR spectrum of complex **3** in CD_2Cl_2 (500 MHz).

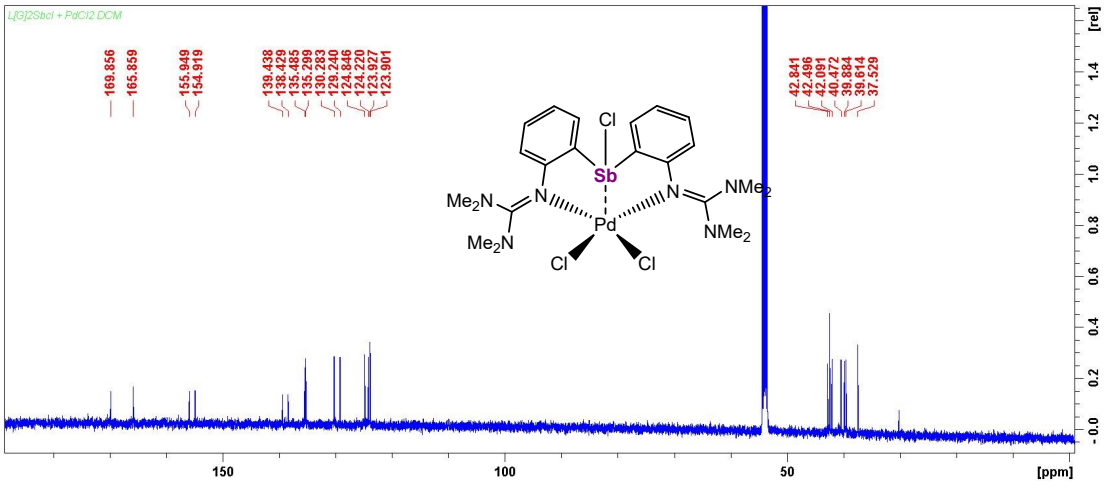


Figure S20: $^{13}C\{^{1}H\}$ NMR spectrum of complex **3** in CD_2Cl_2 (125.6 MHz).

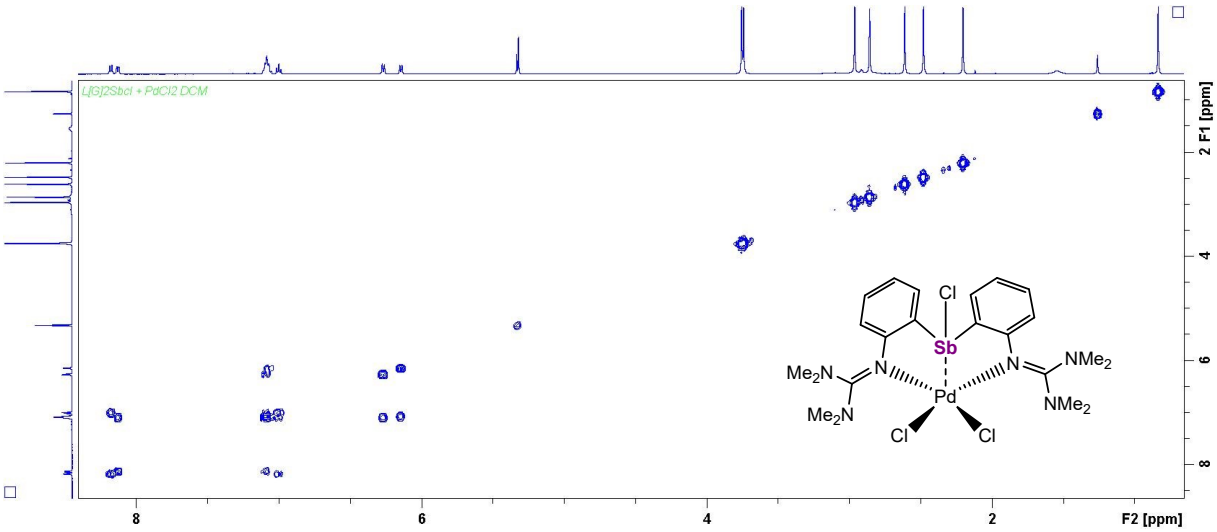


Figure S21: ^{1}H-^{1}H COSY NMR spectrum of complex **3** in CD_2Cl_2 (500 MHz).

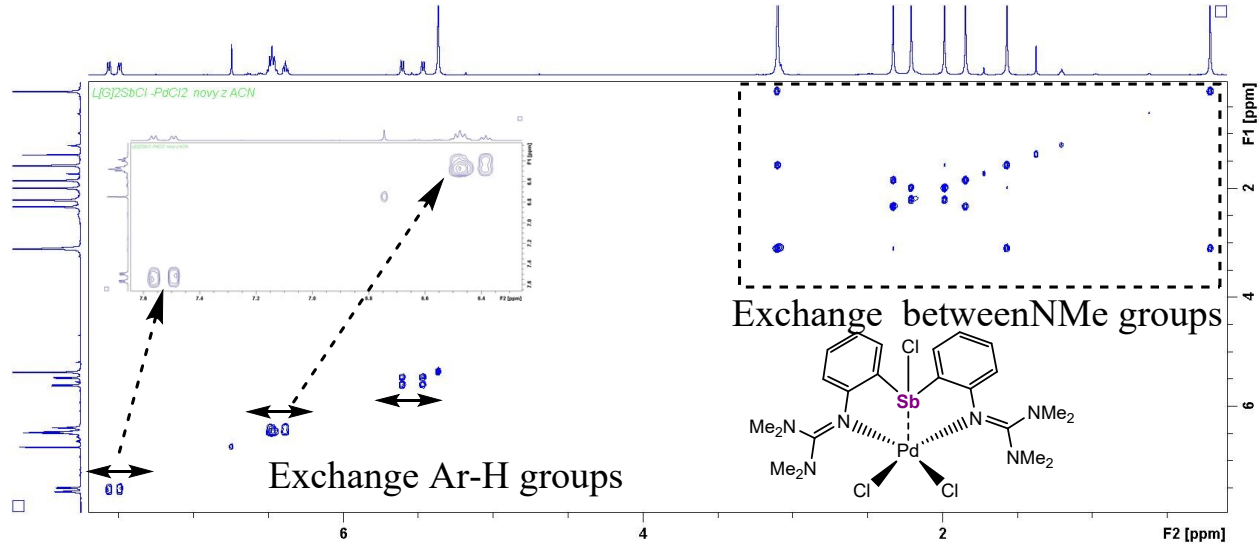


Figure S22: ^{1}H-^{1}H EXSY NMR spectrum of complex **3** in CD_2Cl_2 (mixing time 0.6s, 500 MHz).

2) Crystallography.

Diffraction data for all compounds were collected using a Bruker Venture D8 diffractometer at 150 K with graphite-monochromated Mo-Kα (0.7107 Å) radiation. The frames were integrated with the Bruker SAINT software package using a narrow frame algorithm. Data were corrected for absorption effects using the Multi-Scan method (SADABS). Obtained data were treated by XT-version 2014/5 and SHELXL-2017/1 software implemented in APEX3 v2016.5-0 (Bruker AXS) system.[S2] All non-hydrogen atoms were refined using anisotropic displacement parameters. Hydrogen atoms attached to carbon atoms were included in geometrically calculated positions using a riding model. Furthermore, disorder dichloromethane in **1** and chloroform in **2** were split to two positions by standard methods. Crystallographic data (excluding structure factors) for the structural analyses have been deposited with the Cambridge Crystallographic Data Centre, CCDC nos. 2313661 ($ArSbCl_2$); 2313662 (Ar_2SbCl); 2313664 (Ar_3Sb); 2313665 (**1**); 2313666 (**2**); 2313660 (**3**); 2313659 (**4**). Copies of this information may be obtained free of charge from The Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: +44-1223-336033; e-mail: deposit@ccdc.cam.ac.uk or http://www.ccdc.cam.ac.uk).

Table S1. Crystal data and structure refinement of studied compounds.

	$ArSbCl_2$	**Ar_2SbCl**	**Ar_3Sb**
Formula	$C_{11}H_{16}Cl_2N_3Sb$	$C_{22}H_{32}ClN_6Sb$	$C_{33}H_{48}N_9Sb$
Formula weight, g mol^{-1}	382.92	537.73	692.55
Crystal system	Monoclinic	Monoclinic	Monoclinic
Crystal size, mm	0.59 × 0.24 × 0.11	0.59× 0.45 × 0.39	0.59 × 0.54 × 0.034
Space group	P-2_1/c	P-2_1/n	P-2_1/c
a, Å	8.0916(3)	9.2439(5)	21.8886(9)
b, Å	18.6573(8)	28.6416(13)	14.8090(7)
c, Å	10.0007(4)	9.8442(5)	10.7954(5)
α, º	90	90	90
β, º	105.6870(10)	103.269(2)	90.883(2)
γ, º	90	90	90
V, Å^3	1453.54(10)	2536.8(2)	3498.9(3)
Z	4	4	4
ρ_{calcd}, Mg m^{-3}	1.750	1.408	1.315
μ (Mo $K\alpha$), mm^{-1}	2.249	1.212	0.824
F(000)	752	1096	1440
θ range, deg	1 to 27.5	1 to 30.0	1 to 27.5
No. of reflns collected	34514	67308	69477
No. indep. Reflns	3251	8086	8063
No. obsd reflns with ($I>2\sigma(I)$), R_{int}	3208, 0.011	7236, 0.023	6081, 0.040
No. refined params	158	279	400
GooF (F^2)	1.053	1.180	1.104
R_1 (F) ($I > 2\sigma(I)$)	0.019	0.036	0.042
wR_2 (F^2) (all data)	0.046	0.068	0.061
Largest diff peak/hole, e Å^{-3}	0.424 / –0.590	0.667 / –1.546	0.496 / –1.199
CCDC	2313661	2313662	2313664

$R_{int} = \sum |F_o^2 - F_{o,mean}^2| / \sum F_o^2$, $S = [\sum(w(F_o^2 - F_c^2)^2)/(N_{diffrs} - N_{params})]^{½}$ for all data, $R(F) = \sum ||F_o| - |F_c|| / \sum |F_o|$ for observed data, $wR(F^2) = [\sum(w(F_o^2 - F_c^2)^2)/(\sum w(F_o^2)^2)]^{½}$ for all data.

Table S1 (continuation). Crystal data and structure refinement of studied compounds.

	1	**2**
Formula	$C_{33}H_{48}Cl_2N_9PdSb$ $3(CH_2Cl_2)$	$C_{33}H_{48}Cl_2N_9PtSb$ $CHCl_3$, $2(CH_2Cl_2)$
Formula weight, g mol^{-1}	1124.63	1247.76
Crystal system	Monoclinic	Monoclinic
Crystal size, mm	0.59 × 0.17 × 0.17	0.59 × 0.59 × 0.27
Space group	P-2_1/n	P-2_1/n
a, Å	10.7479(4)	10.7520(3)
b, Å	17.5505(7)	17.4818(6)
c, Å	25.6485(11)	26.1085(10)
α, º	90	90
β, º	94.068(2)	94.0400(10)
γ, º	90	90
V, Å^3	4825.9(3)	4895.3(3)
Z	4	4
ρ_{calcd}, Mg m^{-3}	1.548	1.693
μ (Mo $K\alpha$), mm^{-1}	1.411	3.934
F(000)	2264	2456
θ range, deg	1 to 26.5	1 to 25
No. of reflns collected	110423	100748
No. indep. Reflns	9970	8597
No. obsd reflns with ($I>2\sigma(I)$), R_{int}	8750, 0.017	7836, 0.020
No. refined params	536	515
GooF (F^2)	1.137	1.065
R_1 (F) ($I > 2\sigma(I)$)	0.049	0.038
wR_2 (F^2) (all data)	0.106	0.088
Largest diff peak/hole, e Å^{-3}	1.641 / –1.706	2.147 / –1.780
CCDC	2313665	2313666

$R_{int} = \sum |F_o^2 - F_{o,mean}^2| / \sum F_o^2$, $S = [\sum(w(F_o^2 - F_c^2)^2)/(N_{diffrs} - N_{params})]^{½}$ for all data, $R(F) = \sum ||F_o| - |F_c|| / \sum |F_o|$ for observed data, $wR(F^2) = [\sum(w(F_o^2 - F_c^2)^2)/(\sum w(F_o^2)^2)]^{½}$ for all data.

Table S1 (continuation). Crystal data and structure refinement of studied compounds.

	3	**4**
Formula	$C_{22}H_{32}Cl_3N_6PdSb$	$C_{22}H_{32}Cl_3N_6PtSb$
Formula weight, g mol^{-1}	715.03	803.72
Crystal system	Orthorhombic	Orthorhombic
Crystal size, mm	0.54 × 0.26 × 0.12	0.13 × 0.12 × 0.04
Space group	$P2_12_12_1$	$P2_12_12_1$
a, Å	9.5889(4)	9.5753(3)
b, Å	15.5986(6)	15.6143(5)
c, Å	17.8828(7)	17.9126(5)
α, º	90	90
β, º	90	90
γ, º	90	90
V, Å^3	2674.79(18)	2678.14(14)
Z	4	4
ρ_{calcd}, Mg m^{-3}	1.776	1.993
μ (Mo *K*α), mm^{-1}	2.005	6.549
F(000)	1416	1544
θ range, deg	1 to 28.0	1 to 26.0
No. of reflns collected	25493	23039
No. indep. Reflns	6560	5231
No. obsd reflns with ($I>2\sigma(I)$), R_{int}	6342, 0.029	4782, 0.063
No. refined params	306	307
GooF (F^2)	1.103	0.897
R_1 (F) ($I > 2\sigma(I)$)	0.023	0.028
wR_2 (F^2) (all data)	0.050	0.049
Largest diff peak/hole, e Å^{-3}	0.531 / –0.804	0.683 / –1.003
CCDC	2313660	2313659

$R_{int} = \sum |F_o^2 - F_{o,mean}^2| / \sum F_o^2$, $S = [\sum(w(F_o^2 - F_c^2)^2)/(N_{diffrs} - N_{params})]^{½}$ for all data, $R(F) = \sum ||F_o| - |F_c|| / \sum |F_o|$ for observed data, $wR(F^2) = [\sum(w(F_o^2 - F_c^2)^2)/(\sum w(F_o^2)^2)]^{½}$ for all data.

4) Theoretical study

The calculations were performed using the Gaussian 16 program package.[S3] To obtain NPA charges and Wiberg bond indices, NBO calculations were carried out using the NBO program implemented in Gaussian 16.[S4] The Atoms In Molecules (AIM) Analysis was performed with the MultiWFN program.[S5] The theoretical calculations have been carried using the ωB97X-D range-separated functional, and to test the reliability of this method, the BP86, BP86-D3, B3LYP-D3, and M06-2X functional. The calculated results are in good agreement with the bond distances obtained from the single crystal XRD experiments. Due to the similar results, we only discuss the findings calculated with ωB97X-D/def2-TZVP level.

We examined how strongly the formation of a given complex is preferred thermodynamically. Therefore, we optimized the geometries of artificially generated isomeric model complexes: **1*** and **2***, which contain the triaryl ligand with pentacoordinante Pd and Pt centers, respectively (in similar fashion as in **3** and **4**). Importantly, these isomers have significantly higher relative energies (by 8.2 and 11.0 kcal/mol) compared to the structures containing tetracoordinate metal centers. Similarly, the model complexes **3*** and **4***, in which the Sb center and only one imino-arm of the ligand form dative bonds with the metal centers, also lie remarkably higher in energy (12.9 and 10.3 kcal/mol, compared to **3** and **4**, respectively). These results outline that the formation of complexes having metal centers with given coordination numbers is clearly preferred due to thermodynamic reasons, and inherent stabilization effects determine the stabilities and bonding in these complexes.

Table S2. Properties of the bonds in the complexes calculated distances (d, Å), Wiberg bond indices (WBIs), Electron Density at the Bond Critical Point (ρ, e/Bohr^3) at ωB97X-D/def2-TZVP level.

	M-Sb			**M-Cl**			**M-Cl**			**M-N**		
	d	**WBI**	**ρ**	**d**	**WBI**	**ρ**	**d**	**WBI**	**ρ**	**d**	**WBI**	**ρ**
1	2.480	0.541	0.087	2.387	0.302	0.032	2.297	0.466	0.089	2.131	0.270	0.086
2	2.482	0.610	0.099	2.305	0.523	0.101	2.389	0.341	0.084	2.115	0.328	0.102
3	2.997	0.106	0.029	2.288	0.515	0.092	2.307	0.482	0.088	2.084	0.309	0.092
4	2.946	0.182	0.037	2.301	0.543	0.099	2.316	0.516	0.103	2.076	0.360	0.113
1*	2.485	0.496	0.083	2.352	0.350	0.079	2.283	0.498	0.092	2.138	0.271	0.084
2*	2.480	0.588	0.096	2.360	0.384	0.090	2.296	0.544	0.104	2.122	0.326	0.101
3*	3.175	0.049	0.021	2.294	0.510	0.090	2.315	0.474	0.085	2.091	0.303	0.095
4*	3.184	0.073	0.024	2.308	0.536	0.101	2.321	0.511	0.098	2.086	0.339	0.109

Table S3. Properties of the bonds in the complexes calculated distances (d, Å), Wiberg bond indices (WBIs), Electron Density at the Bond Critical Point (ρ, e/Bohr^3) at ωB97X-D/def2-TZVP level.

	M-N			Cl-Sb		
	d	**WBI**	**ρ**	**d**	**WBI**	**ρ**
3	2.099	0.290	0.097	2.423	0.678	0.078
4	2.088	0.341	0.109	2.455	0.628	0.073
1*	2.104	0.283	0.090		-	
2*	2.077	0.355	0.112		-	
3*		-		2.331	0.769	0.094
4*		-		2.335	0.759	0.093

Table S4. The experimental and calculated bond lengths (Å) in complex **1**

Complex 1						
Bond	**Experimental (XRD)**	**ωB97X-D**	**M06-2X**	**B3LYP-GD3**	**BP86**	**BP86-GD3**
Sb-Pd	2.457	2.480	2.468	2.492	2.51	2.476
N-Pd	2.082	2.131	2.168	2.162	2.13	2.134
Cl-Pd	2.299	2.297	2.332	2.32	2.31	2.315
Cl'-Pd	2.400	2.387	2.438	2.409	2.385	2.394

Table S5. The experimental and calculated bond lengths (Å) in complex **2**

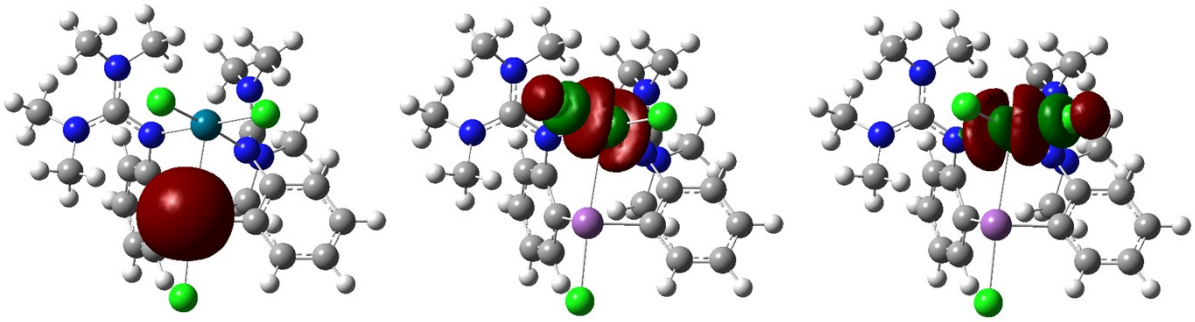
Complex 2						
Bond	**Experimental (XRD)**	**ωB97X-D**	**M06-2X**	**B3LYP-GD3**	**BP86**	**BP86-GD3**
Sb-Pt	2.466	2.482	2.448	2.491	2.510	2.480
N-Pt	2.072	2.115	2.121	2.128	2.114	2.111
Cl-Pt	2.302	2.305	2.316	2.327	2.318	2.319
Cl'-Pt	2.386	2.389	2.436	2.411	2.390	2.401

Table S6. The experimental and calculated bond lengths (Å) in complex **3**

Complex 3						
Bond	**Experimental (XRD)**	**ωB97X-D**	**M06-2X**	**B3LYP-GD3**	**BP86**	**BP86-GD3**
Sb-Cl	2.461	2.423	2.415	2.466	2.495	2.489
Sb-Pd	2.883	2.997	3.066	2.936	2.872	2.866
N-Pd	2.055	2.084	2.109	2.1	2.105	2.082
N'-Pd	2.06	2.099	2.134	2.113	2.115	2.089
Cl-Pd	2.314	2.288	2.336	2.328	2.323	2.325
Cl'-Pd	2.3	2.307	2.307	2.309	2.308	2.305

Table S7. The experimental and calculated bond lengths (Å) in complex **4**

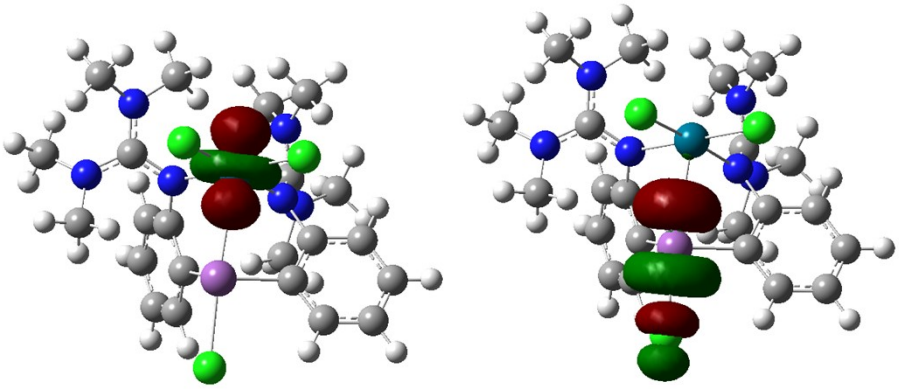
Complex 4						
Bond	**Experimental (XRD)**	**ωB97X-D**	**M06-2X**	**B3LYP-GD3**	**BP86**	**BP86-GD3**
Sb-Cl	2.515	2.455	2.458	2.499	2.522	2.516
Sb-Pt	2.816	2.946	2.931	2.902	2.86	2.857
N-Pt	2.049	2.088	2.093	2.092	2.093	2.077
N'-Pt	2.049	2.076	2.076	2.103	2.102	2.083
Cl-Pt	2.309	2.301	2.327	2.321	2.319	2.317
Cl'-Pt	2.318	2.316	2.304	2.336	2.33	2.331



n_{Sb} $\sigma^*_{Pd\text{-}Cl}$ $\sigma^*_{Pd\text{-}Cl}$

Donor	**Orbital**	**Acceptor**	**Orbital**	**Energy (kcal/mol)**
n_{Sb}	57	$\sigma^*_{Pd\text{-}Cl}$	169	4.08
n_{Sb}	57	$\sigma^*_{Pd\text{-}Cl}$	170	4.06

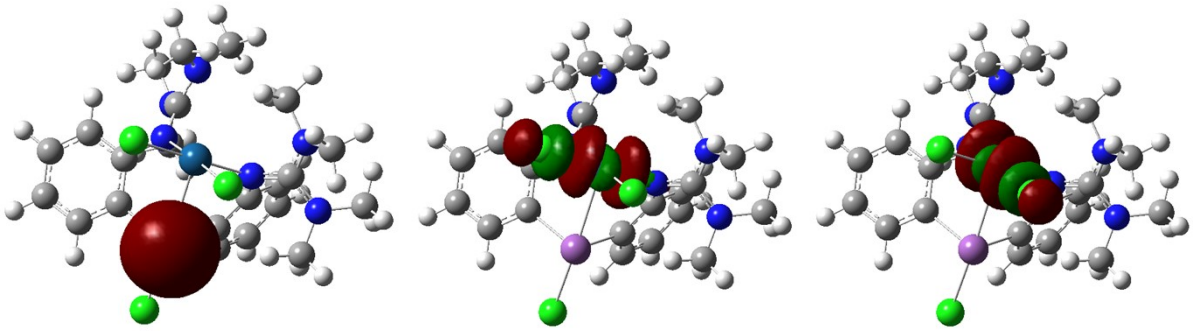
Figure S23. NBOs involved in $n_{Sb} \rightarrow \sigma^*_{Pd\text{-}Cl}$ second order interactions in complex **3**.



n_{Pd} σ^*_{Sb-Cl}

Donor	Orbital	Acceptor	Orbital	Energy (kcal/mol)
n_{Pd}	65	σ^*_{Sb-Cl}	165	10.55

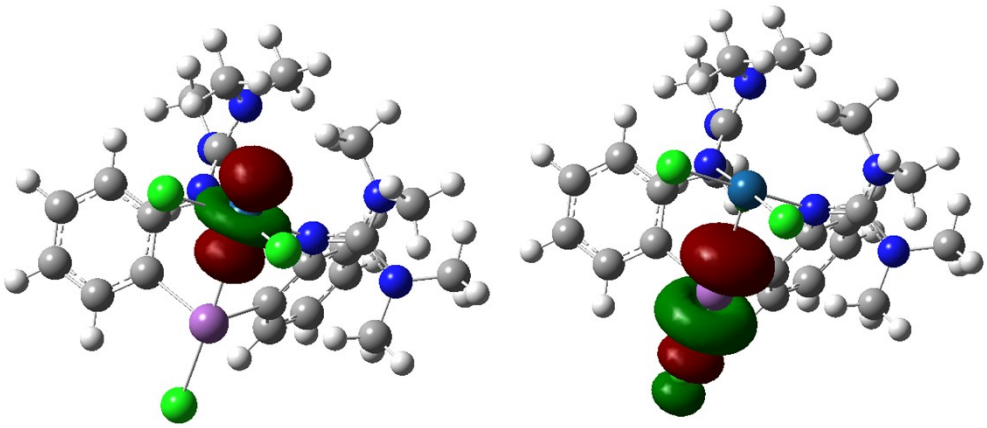
Figure S24. NBOs involved in $n_{Pd} \rightarrow \sigma^*_{Sb-Cl}$ second order interactions in complex **3**.



n_{Sb} σ^*_{Pt-Cl} σ^*_{Pt-Cl}

Donor	Orbital	Acceptor	Orbital	Energy (kcal/mol)
n_{Sb}	57	σ^*_{Pt-Cl}	169	3.80
n_{Sb}	57	σ^*_{Pt-Cl}	170	3.72

Figure S25. NBOs involved in $n_{Sb} \rightarrow \sigma^*_{Pt-Cl}$ second order interactions in complex **4**.



n_{Pt} $\sigma^*_{Sb\text{-}Cl}$

Donor	Orbital	Acceptor	Orbital	Energy (kcal/mol)
n_{Pt}	65	$\sigma^*_{Sb\text{-}Cl}$	165	25.65

Figure S26. NBOs involved in $n_{Pt} \rightarrow \sigma^*_{Sb\text{-}Cl}$ second order interactions in complex **4**.

Table S8. Donor-acceptor interactions in complex **3** and their deletion energies at level ωB97X-D/def2-TZVP.

Interaction	E_{del} (kcal/mol)
$n_{Sb} \rightarrow \sigma^*_{Pd\text{-}Cl}$	5.30
$n_{Pd} \rightarrow \sigma^*_{Sb\text{-}Cl}$	7.87

Table S9. Donor-acceptor interactions in complex **4** and their deletion energies at level ωB97X-D/def2-TZVP.

Interaction	E_{del} (kcal/mol)
$n_{Sb} \rightarrow \sigma^*_{Pt\text{-}Cl}$	4.94
$n_{Pt} \rightarrow \sigma^*_{Sb\text{-}Cl}$	17.90

Geometries:

1

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C -1.845760 4.475183 -1.845085

C -0.470964 4.638152 -1.867953

Sb 1.147529 0.853494 -0.250605

C 2.766611 1.991474 0.651729

N -2.194116 1.112478 -0.339680

Pt -1.411737 -0.663082 -1.081508

Cl -1.811337 0.134377 -3.209303

C 0.268072 0.485370 1.709893

C 0.636913 1.243379 2.817712

C 0.057620 1.054349 4.063510

C -0.933868 0.099173 4.215436

C -1.306542 -0.673151 3.130121

C -0.689857 -0.513943 1.888245

N -1.077645 -1.394924 0.843559

C -0.976922 -2.687825 1.114816

N -1.852995 -3.585258 0.619321

C -3.147000 -3.171278 0.131625

C -3.292758 1.192945 0.381603

N -3.519075 2.168069 1.307480

C -2.449163 2.854505 1.996072

N -4.261465 0.251346 0.250436

C -5.071369 -0.177976 1.366673

C -4.627028 -0.284751 -1.047156

N 0.014417 -3.163860 1.912242

C -0.212073 -4.206553 2.886656

C 1.304783 -2.507455 1.988509

Cl -0.442960 -2.592590 -1.937137

C -4.804290 2.829603 1.387201

C -1.424360 -4.893030 0.162108

H -3.456735 3.150907 -1.383708

H -2.496795 5.230478 -2.267089

H -0.029381 5.525208 -2.303879

H 1.412864 3.755995 -1.432532

H -2.755183 3.023266 3.030672

H -2.218149 3.817332 1.529776

H -1.555910 2.242530 1.996016

H -5.493142 2.418650 0.653645

H -4.672088 3.893987 1.168983

H -5.244966 2.732555 2.383357

H -5.165506 -1.266156 1.339734

H -6.082790 0.242211 1.337701

H -4.597271 0.108084 2.302923

H -4.026403 0.172773 -1.829617

H -5.687302 -0.080813 -1.230966

H -4.467226 -1.363443 -1.090258

H -2.081367 -1.424451 3.235628

H -1.417505 -0.046075 5.173671

H 0.371632 1.660144 4.904041

H 1.399690 2.003120 2.710371

H -3.134307 -3.051242 -0.955287

H -3.416203 -2.220913 0.583586

H -3.886240 -3.930083 0.401615

H -1.938859 -5.689484 0.707241

H -0.351420 -4.999748 0.288463

H -1.644177 -4.981871 -0.903441

H 0.402927 -5.088980 2.686197

H -1.258129 -4.502439 2.886443

H 0.042311 -3.828698 3.881918

H 2.080777 -3.273212 2.050395

H 1.386009 -1.853483 2.861096

H 1.484881 -1.919438 1.093706

C 2.806804 3.328658 1.023730

C 3.933161 3.877901 1.629549

C 5.034365 3.069764 1.877713

C 5.010016 1.727586 1.526011

C 3.885870 1.184472 0.906284

H 1.937584 3.957954 0.869434

H 3.942746 4.922963 1.913538

H 5.916079 3.480980 2.355143

H 5.860759 1.086419 1.732288

N 3.800942 -0.181473 0.622043

C 4.321056 -0.855077 -0.360663

N 4.170299 -2.260681 -0.295365

N 5.016655 -0.367308 -1.445969

C 5.489518 -1.282626 -2.469335

C 4.936068 1.019158 -1.880330

C 3.395090 -2.956617 -1.289611

C 5.056986 -3.013580 0.539546

H 6.288763 -0.794272 -3.023018

H 5.894262 -2.189417 -2.027453

H 4.706502 -1.556742 -3.179624

H 5.770653 1.221174 -2.548527

H 4.005971 1.214858 -2.422238

H 5.002524 1.707002 -1.046718

H 2.776914 -3.718660 -0.807245

H 2.709654 -2.272400 -1.789918

H 4.002473 -3.459689 -2.053450

H 4.554744 -3.925835 0.869811

H 5.991314 -3.315414 0.039816

H 5.312995 -2.429249 1.423646

BH_3

E = -26.6080141

B 0.000000 0.000346 0.000000

H -0.518905 1.074428 0.000000

H 0.259452 -0.538079 1.032984

H 0.259452 -0.538079 -1.032984

3 with BH_3

E = -2961.860198

C -3.848499 -0.791226 -0.924530

C -2.563253 -0.416162 -0.550830

C -2.285836 0.924849 -0.291603

C -3.306232 1.864765 -0.423688

C -4.583621 1.479927 -0.782489

C -4.861240 0.146283 -1.034363

Sb -1.047411 -1.915323 -0.459706

Cl -2.526128 -3.579840 0.390880

N -0.977600 1.362037 0.029365

Pd 0.550605 0.711401 -1.237914

Cl 2.183059 0.027131 -2.699005

C -0.127001 -1.470027 1.426828

C -0.656540 -1.996951 2.600761

C -0.095213 -1.719524 3.836563

C 1.010968 -0.888742 3.907185

C 1.551106 -0.364040 2.747928

C 1.012596 -0.662848 1.492747

N 1.643852 -0.113903 0.355422

C 2.962064 -0.303088 0.286745

N 3.515360 -1.493151 0.621800

C 4.757215 -1.593950 1.355717

N 3.804211 0.674092 -0.089912

C 3.388246 2.055588 -0.095886

C 4.991640 0.398289 -0.878570

C -0.835132 2.276160 0.965561

N 0.135811 3.221994 0.871571

C 0.386500 3.925372 -0.374602

N -1.617555 2.323585 2.077291

C -2.264299 1.151061 2.624508

C -2.133893 3.583837 2.571152

Cl -0.628088 1.613540 -2.979062

C 0.793549 3.758660 2.041389

C 2.802887 -2.736621 0.405900

H -3.077234 2.913626 -0.280671

H -5.357446 2.229176 -0.891891

H -5.854422 -0.162807 -1.332026

H -4.069771 -1.831668 -1.124853

H 1.436356 3.858691 -0.661442

H 0.131731 4.983024 -0.246724

H -0.211529 3.503243 -1.178855

H 1.860570 3.862995 1.832315

H 0.668908 3.081085 2.883237

H 0.414318 4.747730 2.320279

H 4.223905 2.680134 0.228812

H 2.549096 2.181473 0.581699

H 3.083468 2.356884 -1.101946

H 4.925150 0.957989 -1.812596

H 5.036239 -0.656581 -1.130208

H 5.898270 0.689810 -0.341806

H 5.537910 -2.086402 0.769479

H 4.586462 -2.178902 2.264116

H 5.105501 -0.604722 1.642704

H 3.526057 -3.499654 0.114294

H 2.095590 -2.620240 -0.411602

H 2.278645 -3.074307 1.304844

H -1.527300 -2.637160 2.549972

H -0.525950 -2.143564 4.734128

H 1.454487 -0.645410 4.864834

H 2.411852 0.293100 2.799488

H -1.729886 0.258614 2.321601

H -3.305438 1.071083 2.297588

H -2.236578 1.217106 3.714039

H -1.814735 3.774451 3.599396

H -3.227262 3.553465 2.547802

H -1.807137 4.406084 1.939865

B -0.026484 -3.211122 -2.080316

H 0.838328 -2.518657 -2.528350

H 0.296105 -4.096383 -1.322140

H -0.986693 -3.437014 -2.769876

4 with BH_3

E = -2953.3423058

C 3.912028 -0.767107 -0.828601

C 2.616828 -0.412809 -0.472776

C 2.328488 0.916038 -0.172658

C 3.342574 1.867878 -0.251347

C 4.630078 1.502968 -0.595828

C 4.920820 0.180083 -0.885320

Sb 1.079882 -1.897502 -0.471962

Cl 2.601428 -3.599556 0.306423

N 1.006774 1.333670 0.136693

Pt -0.510473 0.619527 -1.095174

Cl 0.642289 1.508817 -2.875393

C 0.208477 -1.570029 1.467614

C 0.769220 -2.147466 2.602353

C 0.238432 -1.928555 3.863612

C -0.867834 -1.106560 4.002928

C -1.439546 -0.530836 2.883483

C -0.929461 -0.772640 1.605964

N -1.588966 -0.174407 0.506281

C -2.910254 -0.364722 0.454816

N -3.761392 0.618725 0.115689

C -3.356554 2.002957 0.143089

C 0.850907 2.250213 1.074448

N 1.609377 2.275919 2.201148

C 2.220508 1.084852 2.750479

N -0.097106 3.213202 0.960891

C -0.765373 3.768623 2.116183

C -0.341889 3.892518 -0.299882

N -3.448868 -1.564910 0.767671

C -4.676063 -1.694711 1.521138

C -2.738559 -2.798102 0.488231

Cl -2.180439 -0.087613 -2.518463

C 2.145929 3.521170 2.711333

C -4.957345 0.355122 -0.663702

H 3.104853 2.910474 -0.078945

H 5.400911 2.260126 -0.664523

H 5.922149 -0.113095 -1.171790

H 4.142304 -1.799344 -1.057249

H 2.176851 1.144488 3.839646

H 3.264615 0.984617 2.439201

H 1.672310 0.206421 2.431236

H 1.849815 4.353862 2.078584

H 3.238472 3.464498 2.707157

H 1.812596 3.713645 3.734546

H -1.825366 3.895656 1.886462

H -0.369219 4.749860 2.397903

H -0.670474 3.092295 2.962941

H 0.292032 3.484856 -1.083296

H -0.127691 4.958923 -0.175229

H -1.380468 3.783705 -0.613879

H -2.299758 0.121030 2.986147

H -1.285447 -0.908726 4.982396

H 0.694330 -2.390768 4.729435

H 1.640341 -2.780334 2.498122

H -3.086334 2.341012 -0.860966

H -2.497090 2.114054 0.796853

H -4.186440 2.609593 0.513566

H -5.857839 0.635782 -0.111262

H -5.003313 -0.695157 -0.933307

H -4.903012 0.931450 -1.588611

H -5.463820 -2.176046 0.935282

H -5.025210 -0.716143 1.841841

H -4.484606 -2.303796 2.409231

H -3.467451 -3.550725 0.184463

H -2.192892 -3.167129 1.361275

H -2.050610 -2.649225 -0.340704

B 0.075353 -3.250347 -2.075883

H -0.802628 -2.583530 -2.534603

H 1.037630 -3.476684 -2.761575

H -0.226308 -4.121123 -1.292823

$SbAr_3$ ligand

E = -2019.542638

C 1.183746 1.336439 1.182351

C 0.204266 0.366397 0.952864

C -0.375952 -0.277188 2.035681

C 0.005641 0.023389 3.335127

C 0.992650 0.973198 3.559051

C 1.585205 1.622356 2.490008

Sb -0.400714 0.122687 -1.097524

C 1.343510 -0.830991 -1.921415

C 1.785710 -0.392266 -3.164060

C 2.913405 -0.928980 -3.769794

C 3.612862 -1.933233 -3.117535

C 3.194831 -2.382913 -1.877731

C 2.068740 -1.831564 -1.254557

N 1.591499 -2.305221 -0.046513

C 2.299687 -2.494815 1.004602

N 1.789293 -3.307860 1.993564

C 1.908779 -2.938166 3.390229

N 1.817524 1.905408 0.079316

C 1.981088 3.166252 -0.089695

N 1.238350 4.173066 0.495030

C -0.125274 3.948967 0.914052

C -1.633072 -1.616615 -0.824049

C -2.858545 -1.378945 -0.189529

C -3.740251 -2.439759 0.031887

C -3.423886 -3.711685 -0.415142

C -2.228596 -3.942632 -1.080972

C -1.339556 -2.894569 -1.277193

N -3.087210 -0.093236 0.297468

C -4.193196 0.547267 0.193927

N -5.193378 0.318331 -0.728494

C -4.904398 -0.267219 -2.016201

N 3.538552 -1.950231 1.277848

C 3.974663 -0.700366 0.704967

C 4.571866 -2.710195 1.938817

N -4.421774 1.600269 1.058739

C -3.495161 1.750761 2.161900

C -4.922122 2.859436 0.543377

N 2.967625 3.590838 -0.955069

C 2.677954 4.623120 -1.931331

C 3.902101 2.586382 -1.423321

C 0.600332 -4.069389 1.675661

C 1.862366 5.364135 1.021753

C -6.589150 0.352298 -0.360562

H -4.668762 -2.258392 0.561586

H -4.113691 -4.528335 -0.237896

H -1.981281 -4.937663 -1.429425

H -0.392203 -3.082496 -1.767178

H -5.571451 3.338145 1.279722

H -5.488186 2.702548 -0.370222

H -4.094486 3.544623 0.318315

H -3.307548 0.787427 2.628256

H -3.934719 2.431200 2.893520

H -2.526558 2.148918 1.837025

H -7.025185 -0.651473 -0.432358

H -7.159707 1.014448 -1.020850

H -6.697635 0.702754 0.662842

H -3.857633 -0.115749 -2.269444

H -5.519230 0.228462 -2.772935

H -5.111236 -1.342357 -2.046426

H 2.369696 2.352643 2.654181

H 1.306596 1.205335 4.569876

H -0.457457 -0.488748 4.169799

H -1.139444 -1.025369 1.863860

H 4.261455 1.994471 -0.585144

H 4.746597 3.093951 -1.892601

H 3.446827 1.899232 -2.145354

H 3.560680 5.244577 -2.097456

H 1.865493 5.257127 -1.588137

H 2.383756 4.179914 -2.890813

H 1.788816 5.380834 2.115959

H 1.379741 6.269135 0.637423

H 2.913928 5.387208 0.746803

H -0.568938 3.144302 0.331096

H -0.700115 4.861650 0.732512

H -0.205881 3.690337 1.975787

H 3.736777 -3.174211 -1.372494

H 4.487856 -2.375001 -3.579724

H 3.234030 -0.576772 -4.742155

H 1.237089 0.391854 -3.677349

H 0.693922 -4.515936 0.689094

H -0.299305 -3.443438 1.668597

H 0.483867 -4.858291 2.421253

H 2.311989 -3.763692 3.984788

H 0.928168 -2.667626 3.792134

H 2.555104 -2.071450 3.500651

H 4.918672 -2.212058 2.851361

H 5.434552 -2.826557 1.271747

H 4.205522 -3.699380 2.201110

H 4.423810 -0.085250 1.491859

H 3.139495 -0.148747 0.285357

H 4.717779 -0.852140 -0.087037

$SbAr_2Cl$ ligand

E = -1886.7353945

C 3.384624 -2.354795 -0.249172

C 2.468521 -1.346772 -0.485762

C 2.891778 -0.022150 -0.624725

C 4.249346 0.283475 -0.577901

C 5.161670 -0.736571 -0.349494

C 4.738747 -2.047009 -0.171841

Sb 0.366046 -1.380550 -0.879645

Cl 0.067177 -3.669982 -0.085326

N 1.837249 0.855909 -0.881263

C -0.223253 -0.532567 1.004663

C 0.479258 -0.765090 2.179073

C 0.104424 -0.163644 3.371517

C -0.987013 0.692825 3.385695

C -1.711637 0.917224 2.227766

C -1.355958 0.286623 1.032060

N -2.084488 0.512617 -0.140514

C -3.346300 0.256109 -0.194842

N -4.113219 0.856681 -1.168019

C -3.537451 1.941282 -1.926964

C 1.710297 2.058642 -0.427570

N 2.432941 2.617368 0.596332

C 2.887694 1.850690 1.731855

N 0.764963 2.873403 -0.999323

C -0.141230 3.623281 -0.146212

C 0.162007 2.439579 -2.243837

N -4.038852 -0.601101 0.634691

C -5.311746 -0.224909 1.205987

C -3.408287 -1.754903 1.239006

C 2.823896 4.007275 0.591886

C -5.123040 0.104038 -1.885600

H 4.586163 1.303183 -0.720826

H 6.219255 -0.504478 -0.312301

H 5.464281 -2.829846 0.009656

H 3.045396 -3.377725 -0.131754

H 2.580697 2.358821 2.651142

H 3.976462 1.737613 1.739264

H 2.436136 0.864375 1.728724

H 2.529987 4.476524 -0.343439

H 3.911466 4.082811 0.695773

H 2.369602 4.561221 1.421189

H -1.085543 3.079722 -0.037310

H -0.341944 4.606834 -0.577376

H 0.281638 3.753869 0.845250

H 0.924981 2.040963 -2.907491

H -0.310358 3.303794 -2.715620

H -0.595633 1.668742 -2.071430

H -2.571395 1.577609 2.237750

H -1.281971 1.183048 4.305766

H 0.664272 -0.354302 4.278338

H 1.337799 -1.428003 2.161802

H -2.882329 1.580848 -2.728716

H -2.949642 2.582085 -1.275295

H -4.345559 2.524486 -2.372922

H -6.032584 0.698062 -2.005145

H -5.368146 -0.807834 -1.349510

H -4.760125 -0.172334 -2.882429

H -6.070328 -0.994511 1.029215

H -5.657620 0.709828 0.771408

H -5.214329 -0.088676 2.289593

H -4.149545 -2.555200 1.304500

H -3.023836 -1.551998 2.243900

H -2.585837 -2.111746 0.623879

$SbAr_3$ligand with BH_3

E = -2046.202253

C	1.005613	1.378363	1.375845
C	0.215896	0.244959	1.169075
C	-0.201639	-0.521310	2.244185
C	0.168974	-0.176822	3.535706
C	0.965988	0.941046	3.745337
C	1.387779	1.714000	2.676919
Sb	-0.367530	-0.087602	-0.841923
C	1.388373	-0.565421	-1.923832
C	1.614322	0.025456	-3.159230
C	2.765740	-0.259130	-3.879450
C	3.693444	-1.146145	-3.351143
C	3.481902	-1.738014	-2.117928
C	2.330550	-1.446716	-1.379321
N	2.023621	-2.052050	-0.173994

C	2.824990	-2.157145	0.824803
N	2.524870	-3.079132	1.800767
C	2.666998	-2.741748	3.204229
N	1.464671	2.049439	0.251306
C	1.322308	3.308220	0.029678
N	0.418739	4.142509	0.642747
C	-0.845725	3.656257	1.144412
C	-1.378711	-1.946415	-0.733951
C	-2.621782	-1.877080	-0.094646
C	-3.398296	-3.032417	0.011442
C	-2.944595	-4.222606	-0.532870
C	-1.718574	-4.284239	-1.181581
C	-0.937094	-3.141133	-1.278992
N	-2.950937	-0.664249	0.494296
C	-4.060611	-0.033882	0.341972
N	-4.979822	-0.233824	-0.657889
C	-4.587781	-0.707070	-1.966115
N	3.966320	-1.417931	1.044600
C	4.133283	-0.081405	0.525380
C	5.155255	-2.006428	1.613998
N	-4.369399	0.963706	1.243872
C	-3.543222	1.050753	2.430178
C	-4.803019	2.257427	0.747032
N	2.125010	3.898255	-0.920790
C	1.522201	4.746340	-1.934353
C	3.249880	3.122906	-1.403702
C	1.470448	-4.029517	1.517825
C	0.742511	5.509016	0.977903
C	-6.401290	-0.142914	-0.423740

H	-4.350795	-2.987344	0.526223
H	-3.553626	-5.114532	-0.445441
H	-1.369509	-5.219174	-1.600945
H	0.029421	-3.185453	-1.766004
H	-5.534545	2.698007	1.428280
H	-5.250713	2.161167	-0.237409
H	-3.949485	2.939771	0.657275
H	-3.402910	0.063447	2.862703
H	-4.045201	1.695391	3.154019
H	-2.549962	1.459834	2.213226
H	-6.879013	-1.102095	-0.652612
H	-6.866530	0.622518	-1.054827
H	-6.594273	0.099920	0.618166
H	-3.543681	-0.471646	-2.153815
H	-5.184820	-0.183074	-2.716794
H	-4.739044	-1.784979	-2.086189
H	2.018175	2.581059	2.835719
H	1.263411	1.212188	4.751369
H	-0.159504	-0.777645	4.374568
H	-0.830973	-1.386167	2.074348
H	3.794297	2.695632	-0.564755
H	3.913662	3.789408	-1.957052
H	2.937214	2.301967	-2.058251
H	2.183226	5.583256	-2.171434
H	0.568722	5.135263	-1.589758
H	1.335651	4.174503	-2.850012
H	0.659615	5.657492	2.060325
H	0.064375	6.216539	0.488091
H	1.761088	5.736943	0.674461

H	-1.151845	2.768706	0.596662
H	-1.604132	4.424854	0.972896
H	-0.815850	3.426510	2.215235
H	4.205095	-2.436382	-1.713247
H	4.591016	-1.385006	-3.909270
H	2.932563	0.198139	-4.846249
H	0.883405	0.718675	-3.561899
H	1.577928	-4.419168	0.508827
H	0.476512	-3.574246	1.592745
H	1.543312	-4.851139	2.232649
H	3.228607	-3.512475	3.740099
H	1.681153	-2.642942	3.667686
H	3.175849	-1.788262	3.316898
H	5.457364	-1.496673	2.535691
H	5.984840	-1.931284	0.901446
H	4.987708	-3.057102	1.836653
H	4.550021	0.553677	1.313652
H	3.181751	0.345891	0.222830
H	4.810915	-0.058067	-0.335931
B	-1.473521	1.561511	-1.913078
H	-0.651699	2.441973	-2.034903
H	-1.792152	1.044556	-2.962303
H	-2.411201	1.847567	-1.204980

$SbAr_2Cl$ ligand with BH_3

E = -1913.365942

C	-0.123961	-0.289417	2.665357
C	0.645269	-0.565127	1.545897
C	1.984425	-0.173421	1.474725

C	2.543643	0.499290	2.566006
C	1.772550	0.766070	3.683203
C	0.439920	0.374782	3.742536
Sb	-0.022251	-1.671422	-0.118796
B	0.672835	-3.763640	-0.587474
N	2.680041	-0.562153	0.344691
C	3.497771	0.186394	-0.312660
N	3.535375	1.562725	-0.280583
C	2.351216	2.349467	-0.033970
C	-2.124837	-1.635707	0.120012
C	-2.823677	-0.432615	0.306948
C	-4.206725	-0.491213	0.509577
C	-4.871319	-1.704539	0.494072
C	-4.181277	-2.889224	0.279299
C	-2.808272	-2.847056	0.092739
N	-2.103466	0.743523	0.378459
C	-2.415959	1.841097	-0.210761
N	-1.861350	3.013540	0.258874
C	-1.182173	2.955992	1.536683
Cl	0.217918	-0.171036	-1.947663
N	-3.241617	1.979051	-1.303298
C	-4.157730	3.088884	-1.431037
C	-3.429302	0.911349	-2.258266
N	4.404533	-0.412389	-1.147188
C	4.646444	0.119461	-2.475044
C	4.563766	-1.849942	-1.049037
C	4.780528	2.294155	-0.283660
C	-1.272879	3.955577	-0.673610
H	-4.750937	0.429457	0.684034

H	-5.942800	-1.725564	0.653451
H	-4.704911	-3.835913	0.265323
H	-2.261173	-3.768763	-0.072611
H	-3.461720	1.342459	-3.262513
H	-4.358104	0.356686	-2.086932
H	-2.594617	0.217014	-2.215454
H	-4.036432	3.774340	-0.596265
H	-5.190746	2.722537	-1.433459
H	-3.994889	3.638579	-2.364373
H	-0.188284	3.806139	-0.739655
H	-1.459088	4.981529	-0.347852
H	-1.689488	3.823140	-1.667744
H	-1.778741	2.396963	2.252776
H	-1.042529	3.975560	1.900484
H	-0.206264	2.462820	1.467052
H	3.585334	0.794961	2.532319
H	2.218606	1.281668	4.525248
H	-0.152556	0.584976	4.623395
H	-1.167015	-0.579550	2.692287
H	3.747074	-2.384836	-1.544314
H	4.575076	-2.153103	-0.005651
H	5.509897	-2.125115	-1.518243
H	5.714067	0.104081	-2.707014
H	4.285004	1.140787	-2.550303
H	4.120270	-0.481748	-3.224229
H	4.836329	2.993371	-1.125126
H	5.619301	1.605629	-0.347633
H	4.876035	2.873119	0.642056
H	2.350008	3.205713	-0.715609

H	2.304141	2.724923	0.994436
H	1.459458	1.759235	-0.231835
H	-0.020616	-4.054022	-1.531761
H	1.854352	-3.682686	-0.785119
H	0.352838	-4.291659	0.456302

PPh_3

E = -1036.3108731

P -0.000000 -0.000000 1.250387

C 1.571348 -0.478673 0.435757

C -0.371131 1.600163 0.435757

C -1.200216 -1.121491 0.435757

C -1.178960 1.742362 -0.688955

C -1.396993 2.993795 -1.246656

C -0.805156 4.118152 -0.692890

C -0.000000 3.988796 0.429464

C 0.205898 2.740655 0.993585

H -1.642228 0.871223 -1.134750

H -2.030321 3.088229 -2.119996

H -0.975212 5.093834 -1.130480

H 0.460571 4.862997 0.872266

H 0.824674 2.647672 1.879191

C 2.270528 -1.548640 0.993585

C 3.454399 -1.994398 0.429464

C 3.969002 -1.361790 -0.692890

C 3.291199 -0.287066 -1.246656

C 2.098410 0.149828 -0.688955

H 1.880614 -2.038025 1.879191

H 3.981194 -2.830364 0.872266

H 4.898996 -1.702359 -1.130480

H 3.689646 0.214195 -2.119996

H 1.575616 0.986600 -1.134750

C -2.476426 -1.192015 0.993585

C -3.454399 -1.994398 0.429464

C -3.163846 -2.756361 -0.692890

C -1.894206 -2.706729 -1.246656

C -0.919450 -1.892190 -0.688955

H -2.705288 -0.609647 1.879191

H -4.441764 -2.032633 0.872266

H -3.923784 -3.391475 -1.130480

H -1.659324 -3.302425 -2.119996

H 0.066613 -1.857823 -1.134750

PPh_3 with BH_3

E = -1062.98111862

P 0.000000 -0.000000 0.959208

C -1.575216 -0.538612 0.236743

C 1.254060 -1.094871 0.236743

C 0.321156 1.633483 0.236743

C 1.946046 -0.775379 -0.927472

C 2.875662 -1.660265 -1.451804

C 3.119567 -2.868388 -0.817428

C 2.437147 -3.189434 0.346856

C 1.510473 -2.306241 0.875345

H 1.765964 0.169716 -1.424219

H 3.412338 -1.402279 -2.355887

H 3.847347 -3.557784 -1.226553

H 2.632042 -4.127757 0.850128

H 0.989041 -2.548831 1.792707

C -2.752500 -0.154987 0.875345

C -3.980704 -0.515914 0.346856

C -4.043880 -1.267430 -0.817428

C -2.875662 -1.660265 -1.451804

C -1.644521 -1.297636 -0.927472

H -2.701873 0.417881 1.792707

H -4.890764 -0.215537 0.850128

H -5.004805 -1.553008 -1.226553

H -2.920578 -2.254032 -2.355887

H -0.736003 -1.614228 -1.424219

C 1.242027 2.461228 0.875345

C 1.543557 3.705348 0.346856

C 0.924314 4.135818 -0.817428

C -0.000000 3.320529 -1.451804

C -0.301525 2.073015 -0.927472

H 1.712832 2.130950 1.792707

H 2.258721 4.343294 0.850128

H 1.157458 5.110792 -1.226553

H -0.491760 3.656311 -2.355887

H -1.029961 1.444512 -1.424219

B 0.000000 -0.000000 2.878455

H 1.129791 0.299259 3.196907

H -0.824061 0.828798 3.196907

H -0.305729 -1.128057 3.196907

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