Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary material for:

Synthesis and non-conventional structure of square-planar Pd(II) and Pt(II) complexes with an *N,C,N*-chelated stibinidene ligand

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Table S1. Relevant crystallographic data for the studied compounds.

	1	***anti*-2**	***anti*-3**
chemical formula	$C_{18}H_{29}Cl_2N_2PtSSb$	$C_{18}H_{29}Cl_2N_2OPtSSb\cdot CH_2Cl_2$	$C_{25}H_{35}ClN_3PdSb\cdot 0.25(C_7H_8)$
Cryst syst	monoclinic	monoclinic	triclinic
Space group	*P2₁/c*	*P2₁/c*	*P-1*
a[Å]	11.7080(7)	9.6040(8)	10.4060(11)
b[Å]	15.1261(12)	16.5811(19)	15.3330(8)
c[Å]	14.1141(10)	17.4040(4)	18.462(2)
α[°]	90	90	76.301(8)
β[°]	116.630(7)	104.845(5)	75.302(9)
γ[°]	90	90	88.858(7)
Z	4	4	4
μ[mm^{-1}]	7.800	6.715	1.742
D_x [Mg m^{-3}]	2.061	1.969	1.595
Cryst size [mm]	0.33x0.30x0.08	0.58×0.28×0.22	0.41x0.31x0.12
θ range, [deg]	1-27.5	1-27.5	1-27.5
T_{min}, T_{max}	0.177, 0.571	0.120, 0.320	0.589, 0.827
no. of reflns measd	19827	18710	53 711
no. of unique reflns, R_{int}	5119, 0.032	6021, 0.069	12626, 0.047
no. of obsd reflns	4339	5337	9391
no. of params	226	262	559
S all data	1.092	1.103	1.146
final R indices [$I>2\sigma(I)$]	0.028	0.056	0.047
wR2 indices (all data)	0.055	0.139	0.104
Δρ, max., min. [e $Å^{-3}$]	2.345, -1.756	2.900, -6.037	1.472, -1.711

	***anti*-4**	***syn*-5**	***syn*-6**
chemical formula	$C_{25}H_{35}ClN_3PtSb\cdot 0.25(C_7H_8)$	$C_{29}H_{39}ClFeN_3PdSb\cdot C_7H_8$	$C_{29}H_{39}ClFeN_3PtSb\cdot C_7H_8$
Cryst syst	triclinic	monoclinic	monoclinic
Space group	*P-1*	*P2₁/c*	*P2₁/c*
a[Å]	10.4290(7)	13.4300(14)	13.4290(9)
b[Å]	15.2980(19)	13.5021(15)	13.4550(14)
c[Å]	18.435(3)	19.250(2)	19.273(2)
α[°]	76.369(11)	90	90
β[°]	75.412(9)	95.129(11)	95.323(7)
γ[°]	88.802(7)	90	90
Z	4	4	4
μ[mm^{-1}]	6.149	1.801	5.317
D_x [Mg m^{-3}]	1.809	1.607	1.781
Cryst size [mm]	0.59x0.29x0.25	0.25x0.16x0.13	0.47x0.15x0.03
θ range, [deg]	1-27.5	1-27.5	1-27.5
T_{min}, T_{max}	0.133, 0.399	0.668, 0.795	0.319, 0.850
no. of reflns measd	44 316	29 931	151 039
no. of unique reflns, R_{int}	12043, 0.030	7909, 0.061	33559, 0.070
no. of obsd reflns	10300	6321	7935
no. of params	559	407	388
S all data	1.118	1.244	1.201
final R indices [$I>2\sigma(I)$]	0.035	0.086	0.059
wR2 indices (all data)	0.089	0.186	0.118
Δρ, max., min. [e $Å^{-3}$]	2.766, -2.939	1.484, -1.480	3.975, -2.058

Definitions: $R_{int} = \sum | F_o^2 - F_{o,mean}^2 | / \sum F_o^2$, $S = [\sum(w(F_o^2 - F_c^2)^2)/(N_{diffrs} - N_{params})]^{½}$ 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.

Assignment of *syn* – *anti* rotamers of compound 2 utilizing ^{1}H-^{1}H NOESY

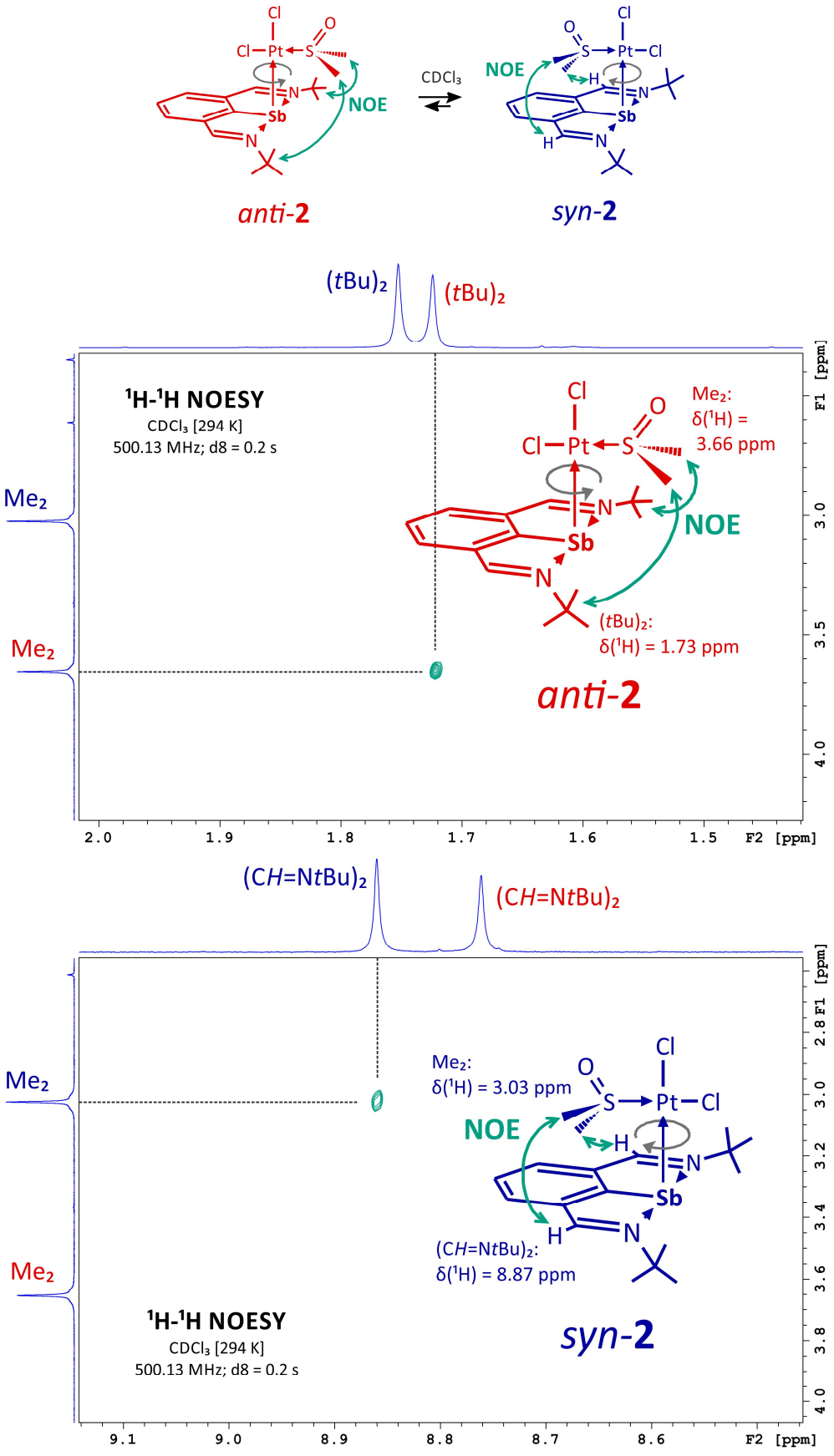

Figure S1. ^{1}H-^{1}H NOESY of compound **2**.

Experimental determination of *syn*-2 – *anti*-2 activation parameters

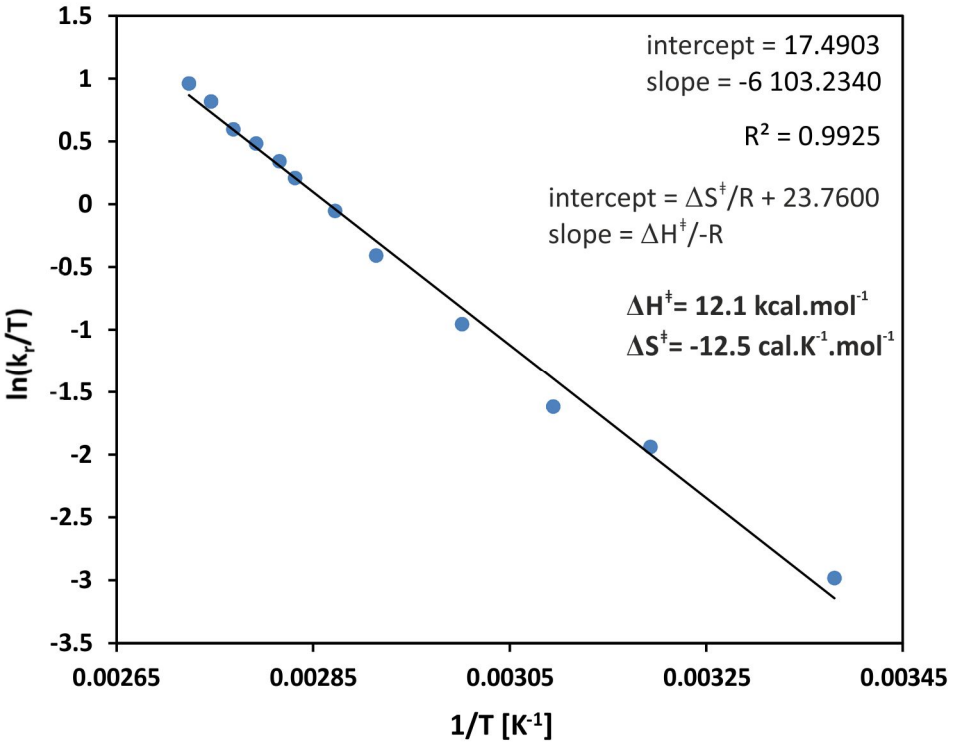

Figure S2. Eyring plot of data of compound **2** obtained from ^{1}H VT-NMR spectra (400.13 MHz) in $C_2Cl_4D_2$ and rates extracted from DNMR3 simulation (based on coalescence of Me_2SO methyl groups).

Computational results

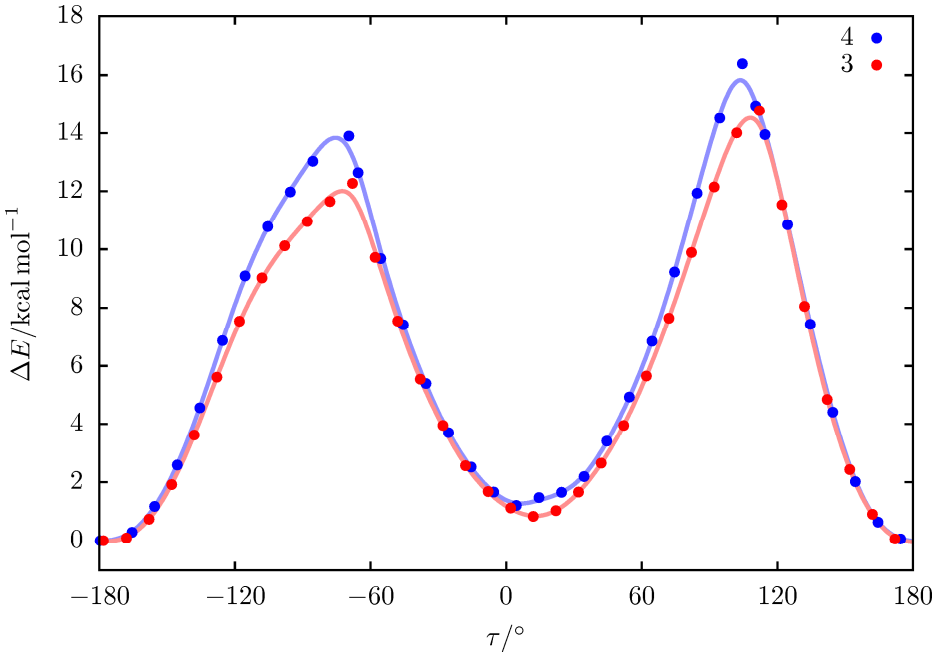

Figure S3. Least energy profile for the torsion angle Cl(1)-M(1)-Sb(1)-C(1) for compounds **3** and **4** (with M being Pd and Pt, respectively).

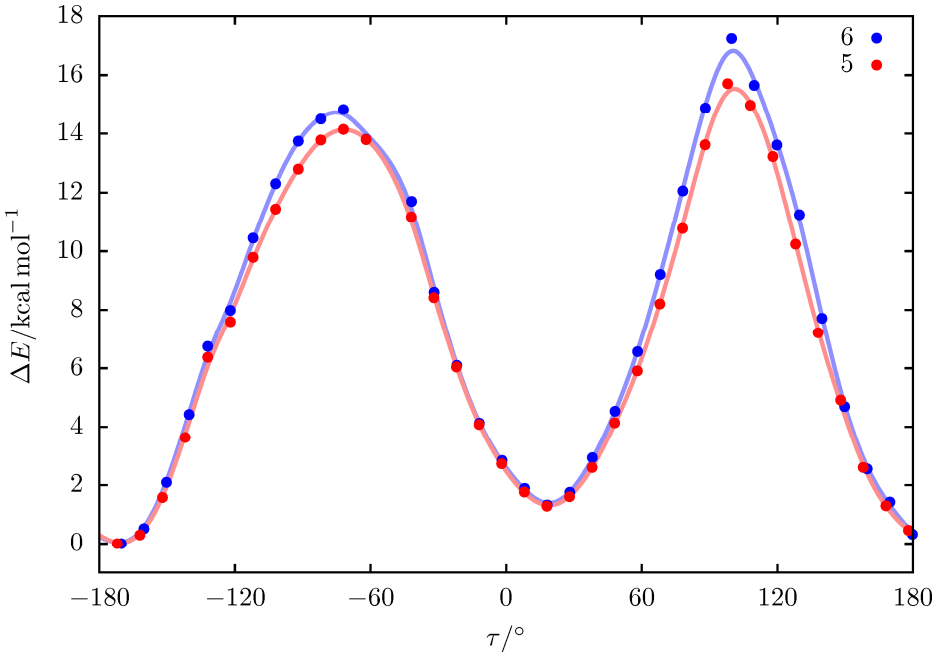

Figure S4. Least energy profile for the torsional angle Cl(1)-M(1)-Sb(1)-C(1) for compounds **5** and **6** (with M being Pd and Pt, respectively).

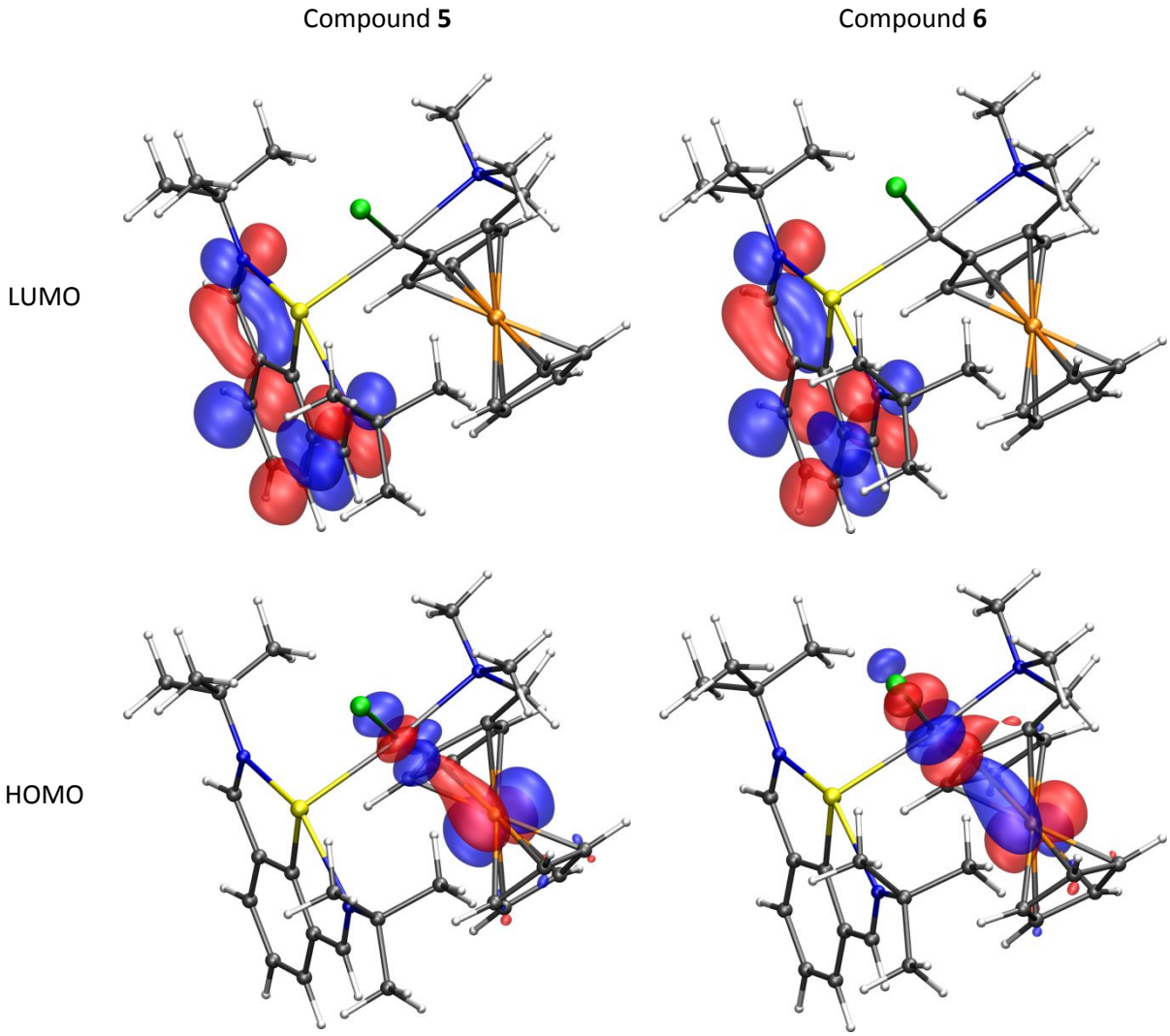

Figure S5. Highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbitals (LUMO) for compounds **5** and **6** (isosurface of 0.05 a.u.). Color code: C – black, H – white, Sb – yellow, Pd/Pt – gray, Fe – orange, and Cl – green.