Electronic Supplementary Information for

Metal-metal multiple bond formation induced by σ-acceptor Lewis acid ligands

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General considerations

All operations were performed under an inert atmosphere of nitrogen or argon using standard Schlenk line or glovebox techniques, employing dry solvents and glassware unless otherwise noted. The starting material [Cp*Ru(μ-NHPh)]$_2$ (**1**) was prepared as described previously.[1] Deuterated solvents were degassed by freeze-pump-thaw cycles and stored over molecular sieves which had been dried at 300 °C under vacuum overnight. Other reagents and solvents were purchased from commercial venders and used as received. NMR spectra were obtained on a JEOL JNM-AL400 or a ECP400 spectrometers at 22 °C unless otherwise specified. Variable-temperature ^{1}H NMR spectra were obtained on a JEOL ECZ500R spectrometer. Elemental analyses were performed on a Perkin Elmer 2400 Series II analyzer.

Experimental procedure and characterization data

Synthesis of [(Cp*Ru)$_2$(μ-NHPh)$_2$ZnCl$_2$] (2)

Complex **1** (215 mg, 0.327 mmol) was placed in a Schlenk tube and dissolved in THF (15 mL). The solution was cooled to −80 °C with a hexane-liquid N_2 bath and treated with a slurry of $ZnCl_2$ (44.6 mg, 0.327 mmol) in THF (5 mL) via a Teflon tubing. The resulting mixture was warmed slowly to room temperature and stirred for 3 h, giving a dark red solution. The solvent was removed in vacuo, and the residue was extracted with CH_2Cl_2 (10 mL). The extract was filtered into a clean Schlenk tube through a Teflon tubing fitted with a plug of filter paper at one end, concentrated to ca. 2 mL under reduced pressure, and layered with hexane (8 mL). The red crystalline solid that deposited was collected by filtration and dried in vacuo. Yield: 211 mg (0.266 mmol, 81%). Anal. Calcd. for $C_{32}H_{42}Cl_2N_2Ru_2Zn$: C, 48.46; H, 5.34; N, 3.53. Found: C, 48.28; H, 5.38; N, 3.42. ^{1}H NMR(400 MHz, CD_2Cl_2): δ 8.76 (br s, 2H, NH), 7.37 (m, 4H, Ph), 7.21 (m, 2H, Ph), 7.13 (m, 2H, Ph), 7.05 (m, 2H, Ph), 1.41 (s, 30H, Cp*). ^{13}C{^{1}H} NMR (100 MHz, CD_2Cl_2): δ 156.0, 129.9, 128.4, 126.3, 124.4, 120.6 (Ph), 94.2 (C_5Me$_5$), 9.3 (C$_5$*Me*$_5$). Single-crystals suitable for X-ray analysis were grown from THF-hexane.

Synthesis of [(Cp*Ru)$_2$(μ-NHPh)$_2$PbCl$_2$] (3)

A solution of **1** (1.76 g, 2.69 mmol) in THF (20 mL) was transferred via a Teflon tubing to a stirred slurry of $PbCl_2$ (3.81 g, 13.7 mmol) in THF (5 mL). The resulting mixture was stirred at room temperature for 3 h, giving a dark brown suspension. The solvent was removed in vacuo, and the residue was extracted with CH_2Cl_2 (30 mL). The extract was filtered into a clean Schlenk tube through a Teflon tubing fitted with a plug of Celite at one end, concentrated to ca. 6 mL under reduced pressure, layered with acetonitrile (24 mL), and stored in a freezer (−30 °C). The black plates that deposited were collected by filtration and dried in vacuo. Yield: 1.82 g (1.95 mmol, 72%). Anal. Calcd. for $C_{32}H_{42}Cl_2N_2PbRu_2$: C, 41.11; H, 4.53; N, 3.00. Found: C, 41.26; H, 4.84; N, 2.73. ^1H NMR (400 MHz, $CDCl_3$): δ 13.54 (br s, 2H, NH), 7.98 (m, 2H, Ph), 6.89 (m, 2H, Ph), 7.32 (m, 4H, Ph), 7.20 (m, 2H, Ph), 1.11 (s, 30H, Cp*). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 156.6, 129.5, 128.6, 125.7, 124.8, 122.8 (Ph), 96.0 (C_5Me_5), 7.7 (C_5Me_5). Single-crystals suitable for X-ray analysis were grown from CH_2Cl_2-acetonitrile.

Synthesis of [(Cp*Ru)$_2$(μ-NHPh)$_2$SnCl(OTf)] (4)

Complex **1** (151 mg, 0.211 mmol) was placed in a Schlenk tube and dissolved in THF (10 mL). The solution was cooled to −80 °C with a hexane-liquid N_2 bath and treated with a solution of $SnCl_2$ (40 mg, 0.211 mmol) in THF (5 mL) via a syringe. After 5 minutes, a solution of NaOTf (500 mg, 2.91 mmol) in THF (10 mL) was added dropwise to the reaction solution. The resulting greenish brown mixture was then slowly warmed to room temperature and stirred for 3 h. The solvent was removed in vacuo, and the residue was extracted with CH_2Cl_2 (15 mL). The extract was filtered into a clean Schlenk tube through a Teflon tubing fitted with a plug of filter paper at one end, concentrated to ca. 3 mL under reduced pressure, and layered with hexane (9 mL). The black blocks that deposited were collected by filtration and dried in vacuo. Yield: 128 mg (0.133 mmol, 79%). Anal. Calcd. for $C_{33}H_{42}ClF_3N_2O_3Ru_2SSn$: C, 41.29; H, 4.41; N, 2.92. Found: C, 41.46; H, 4.43; N, 2.76. ^1H NMR(400 MHz, CD_2Cl_2): δ 11.98 (br, 2H, NH), 7.90 (m, 2H, Ph), 7.42 (m, 2H, Ph), 7.35 (m, 2H, Ph), 7.24 (m, 2H, Ph), 6.70 (m, 2H, Ph), 1.16 (s, 30H, Cp*). $^{13}C\{^1H\}$ NMR (100 MHz, CD_2Cl_2): δ 156.5, 130.2, 129.2, 125.8, 125.4, 122.4 (Ph), 121.1 (q, J = 320 Hz, CF_3), 96.7 (C_5Me_5), 8.4 (C_5Me_5). ^{19}F NMR (376 MHz, CD_2Cl_2): δ −78.4 (s, CF_3SO_3). Single-crystals suitable for X-ray analysis were grown from CH_2Cl_2-hexane.

Synthesis of [(Cp*Ru)$_2$(μ-NHPh)$_2$Sn(OTf)$_2$] (5)

Complex **1** (132 mg, 0.201 mmol) was placed in a Schlenk tube and dissolved in THF (6 mL). To this solution was added a solution of $Sn(OTf)_2$ (83.8 mg, 0.201 mmol) in THF (4 mL) by a syringe. The resulting greenish brown solution was stirred at room temperature for 15 min. The solvent was removed in vacuo, and the residue was recrystallized from CH_2Cl_2-hexane (2 mL/7 mL). The black plates that deposited were collected by filtration and dried in vacuo. Yield: 178 mg (0.165 mmol, 82%). Anal. Calcd. for $C_{34}H_{42}F_6N_2O_6Ru_2S_2Sn$: C, 38.04; H, 3.94; N, 2.61. Found: C, 37.88; H, 3.68; N, 2.48. [1]H NMR(400 MHz, CD_2Cl_2): δ 11.67 (br s, 2H, NH), 7.73 (m, 2H, Ph), 7.40 (m, 4H, Ph), 7.32 (m, 2H, Ph), 6.70 (m, 2H, Ph), 1.20 (s, 30H, Cp*). [13]C{[1]H} NMR (100 MHz, CD_2Cl_2): δ 155.8, 130.4, 129.6, 126.3, 125.1, 122.3 (Ph), 120.2 (q, J = 320.5 Hz, CF_3), 97.9 (*C*$_5$Me$_5$), 8.3 (C$_5$*Me*$_5$). [19]F NMR (376 MHz, CD_2Cl_2): δ −78.1 (s, CF_3SO_3). Single-crystals suitable for X-ray analysis were grown from CH_2Cl_2-hexane.

NMR spectra of new compounds

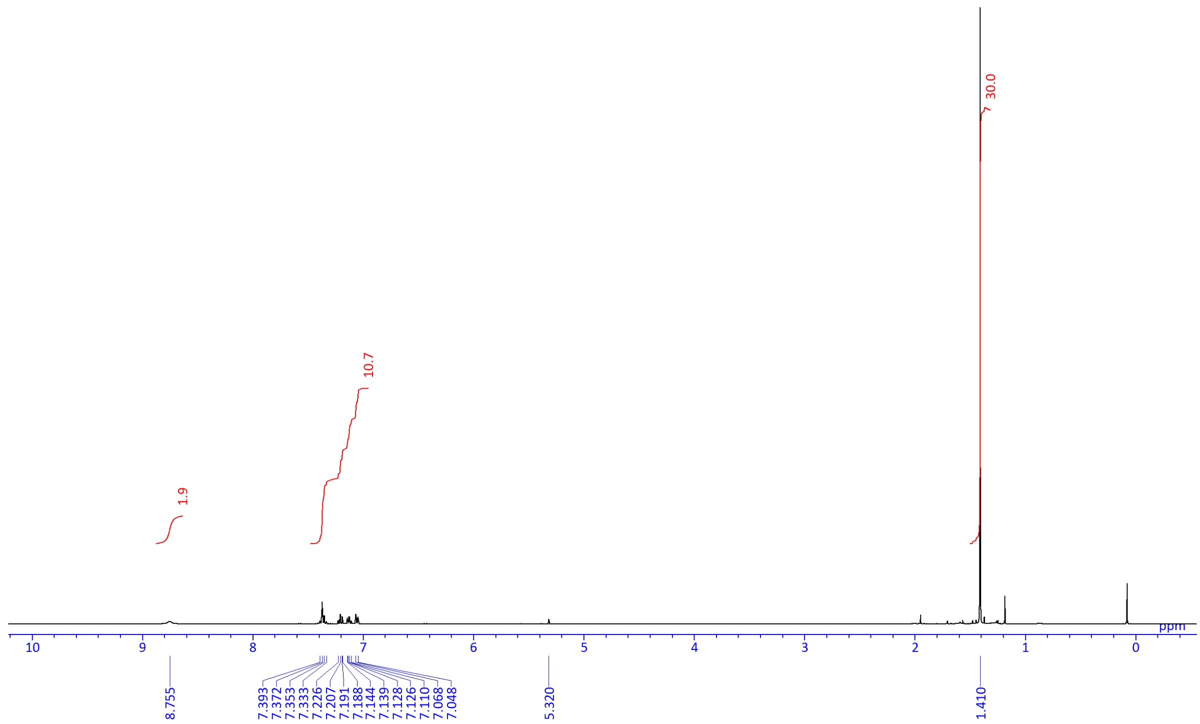


Fig. S1 [1]H NMR spectrum of [(Cp*Ru)$_2$(μ-NHPh)$_2$ZnCl$_2$] (**2**) (400 MHz, CD_2Cl_2).

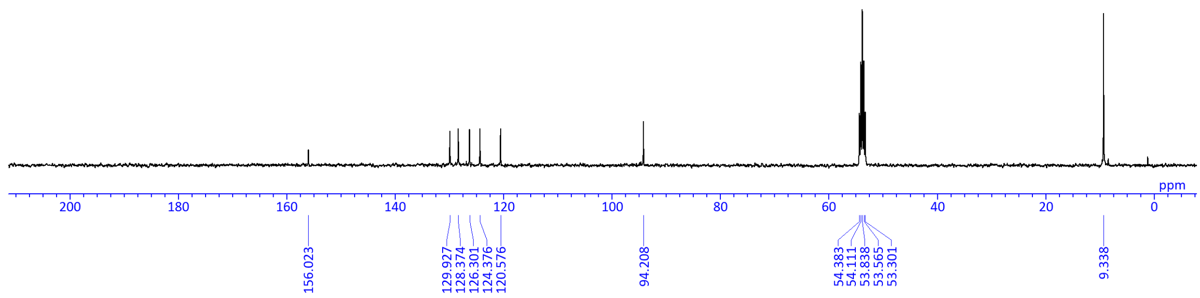


Fig. S2 [13]C{[1]H} NMR spectrum of [(Cp*Ru)$_2$(μ-NHPh)$_2$ZnCl$_2$] (**2**) (100 MHz, CD_2Cl_2).

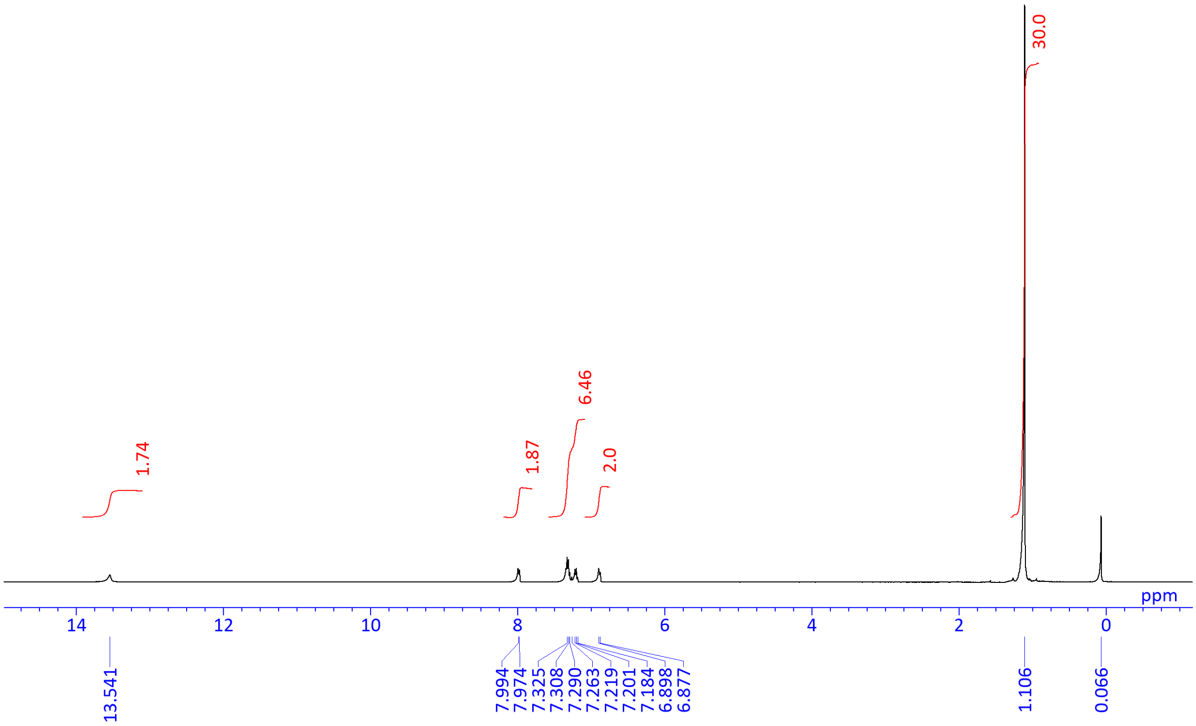


Fig. S3 ^{1}H NMR spectrum of [(Cp*Ru)$_2$(μ-NHPh)$_2$PbCl$_2$] (**3**) (400 MHz, $CDCl_3$).

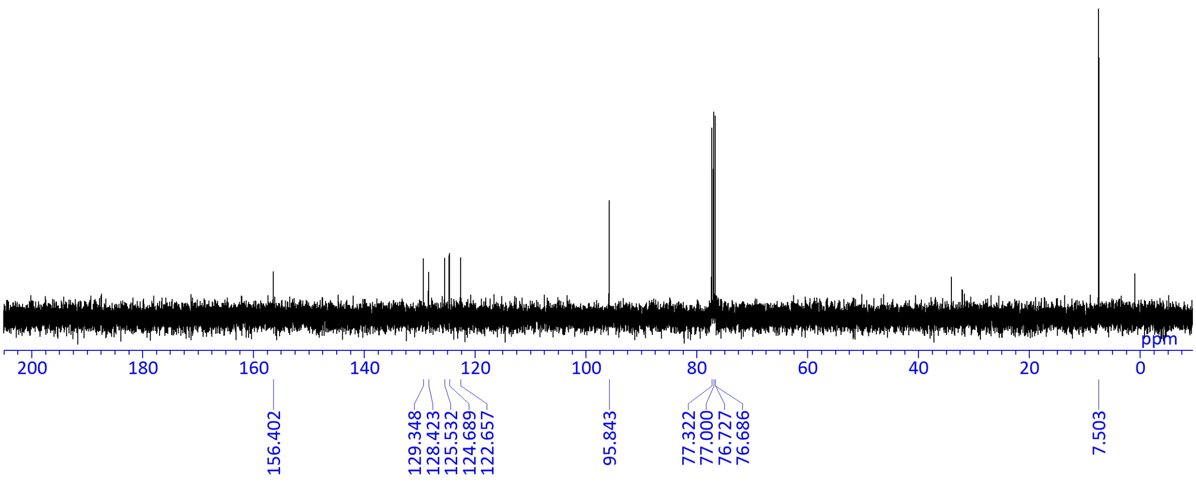


Fig. S4 $^{13}C\{^{1}H\}$ NMR spectrum of [(Cp*Ru)$_2$(μ-NHPh)$_2$PbCl$_2$] (**3**) (100 MHz, $CDCl_3$).

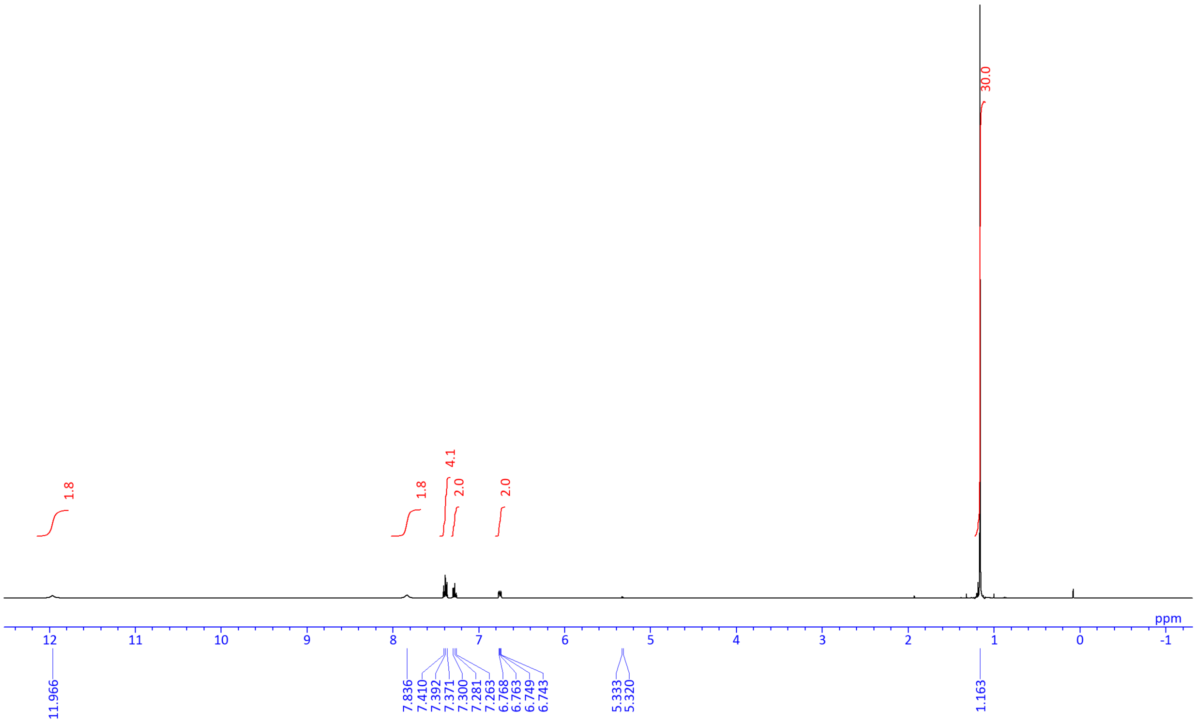


Fig. S5 ^{1}H NMR spectrum of [(Cp*Ru)$_2$(μ-NHPh)$_2$SnCl(OTf)] (**4**) (400 MHz, CD_2Cl_2).

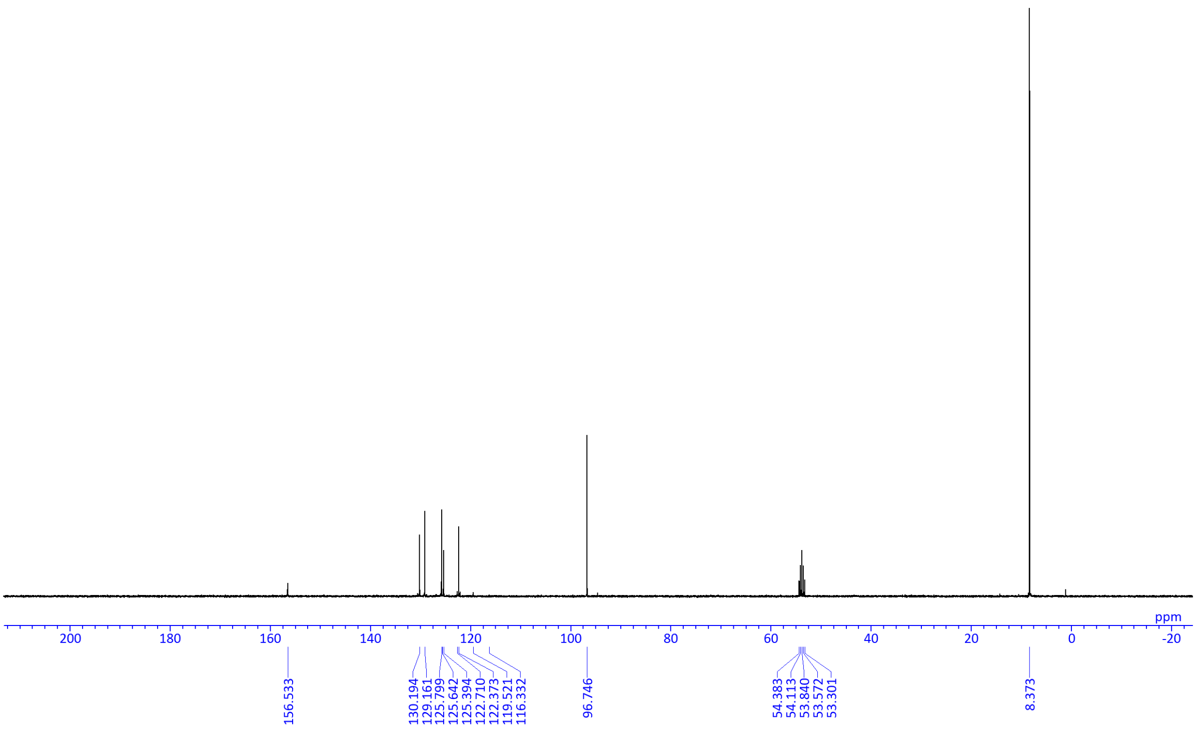


Fig. S6 $^{13}C\{^{1}H\}$ NMR spectrum of [(Cp*Ru)$_2$(μ-NHPh)$_2$SnCl(OTf)] (**4**) (100 MHz, CD_2Cl_2).

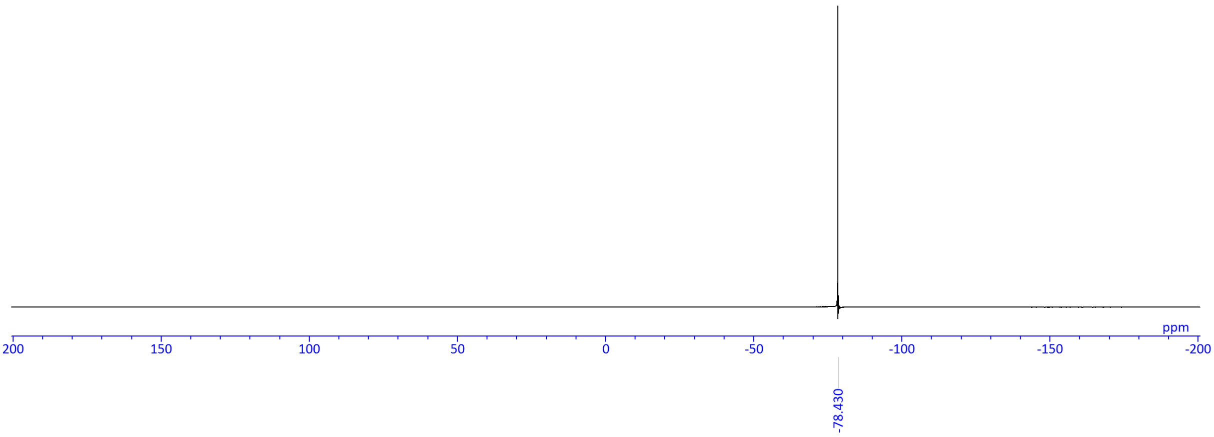


Fig. S7 ^{19}F NMR spectrum of [(Cp*Ru)$_2$(μ-NHPh)$_2$SnCl(OTf)] (**4**) (376 MHz, CD_2Cl_2).

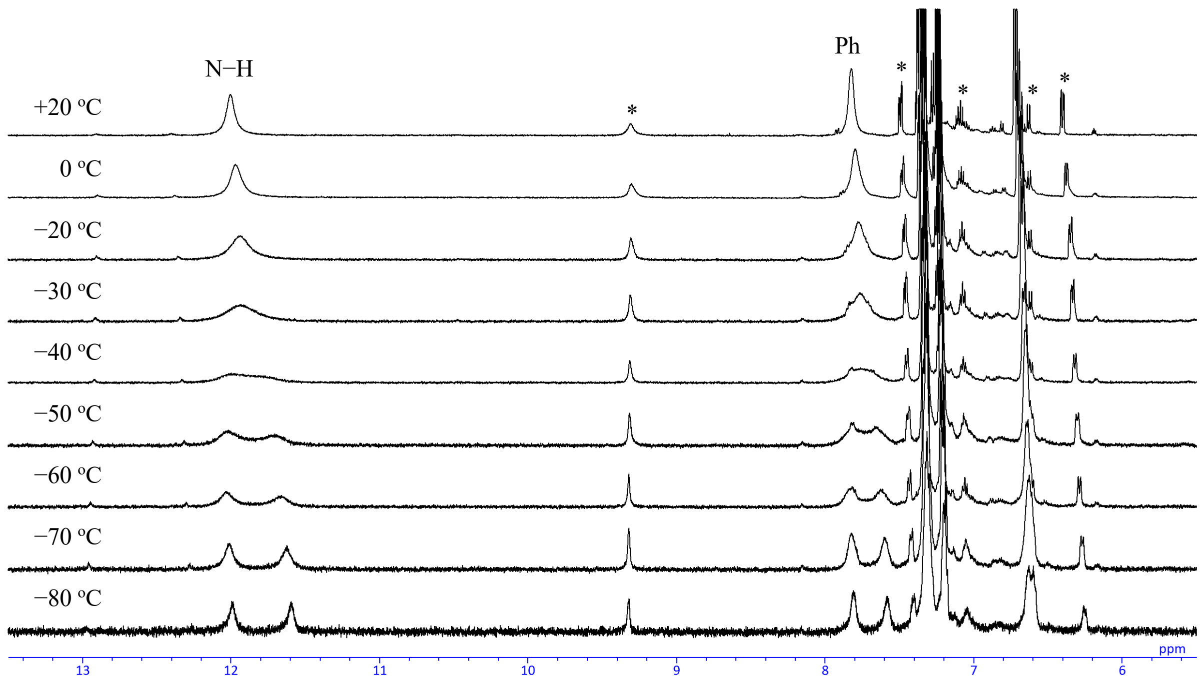


Fig. S8 Variable-temperature ^{1}H NMR spectra of [(Cp*Ru)$_2$(μ-NHPh)$_2$SnCl(OTf)] (**4**) (500 MHz, CD_2Cl_2, NH and aromatic region). Asterisks denote impurities.

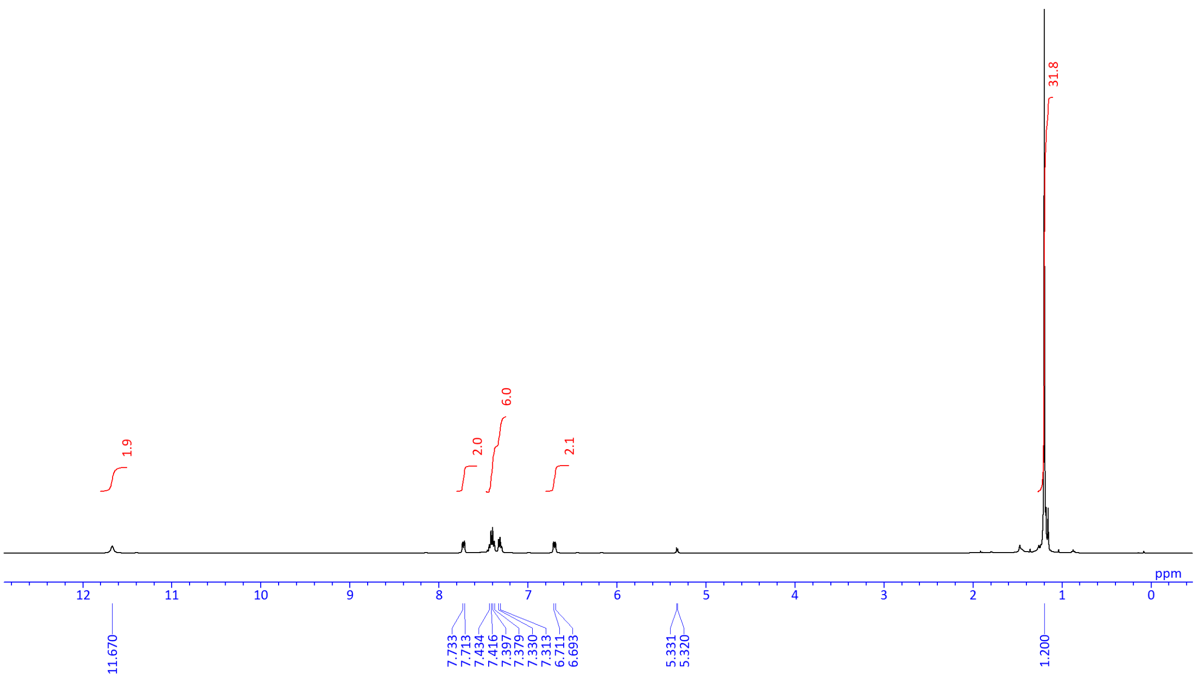


Fig. S9 ^{1}H NMR spectrum of [(Cp*Ru)$_2$(μ-NHPh)$_2$Sn(OTf)$_2$] (**5**) (400 MHz, CD_2Cl_2).

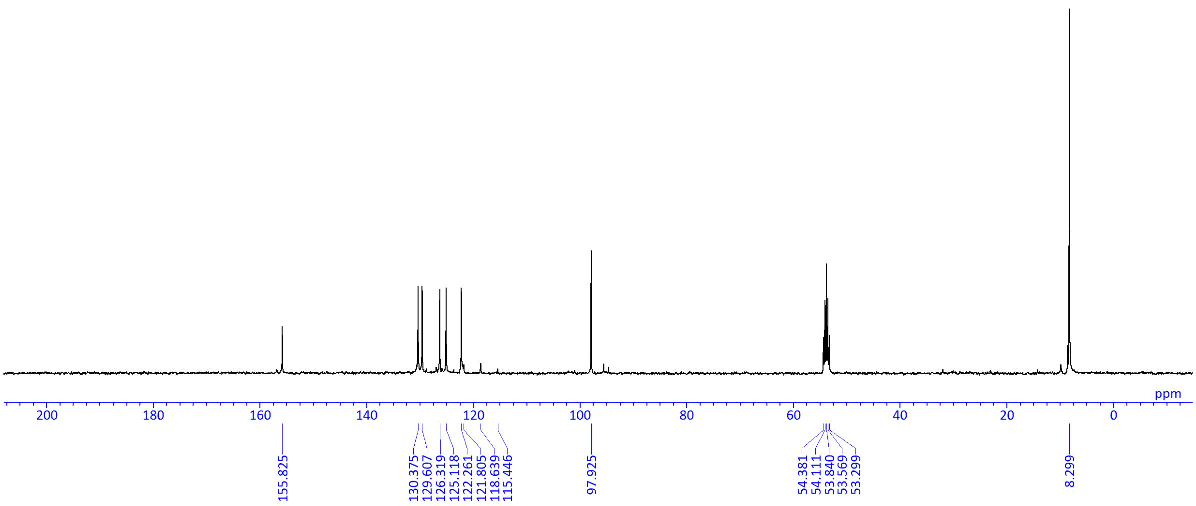


Fig. S10 $^{13}C\{^{1}H\}$ NMR spectrum of [(Cp*Ru)$_2$(μ-NHPh)$_2$Sn(OTf)$_2$] (**5**) (100 MHz, CD_2Cl_2).

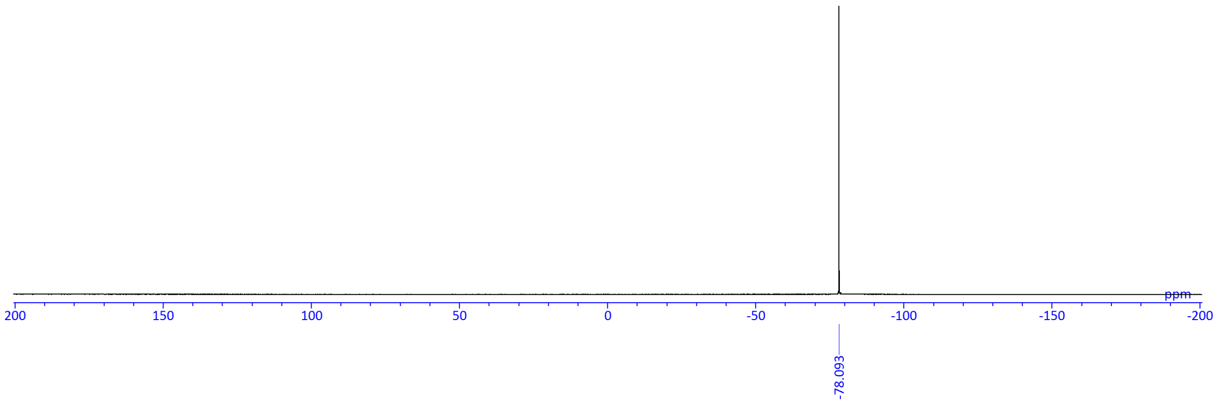


Fig. S11 [19]F NMR spectrum of $[(Cp^*Ru)_2(\mu\text{-}NHPh)_2Sn(OTf)_2]$ (**5**) (376 MHz, CD_2Cl_2).

X-ray crystallography

Single crystals of each compound were prepared as described in the synthetic procedures. All measurements were performed on a Rigaku R-AXIS Rapid imaging plate detector with graphite monochromated Mo Kα radiation (λ = 0.71069 Å). The frame data were processed using Rigaku PROCESS-AUTO,[2] and the reflection data were corrected for absorption with ABSCOR.[3] The structures were solved by SHELXS-97 and refined by SHELXL-97.[4] All non-hydrogen atoms were refined with anisotropic displacement parameters unless otherwise mentioned. Hydrogen atoms were placed at calculated positions and treated as riding models unless otherwise mentioned. Selected crystallographic data are summarized in Table S1. CCDC 2041261-2041264.

Table S1 Crystallographic data for **2**, **3**, **4** and **5**.

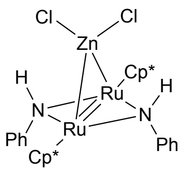
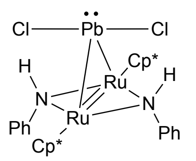
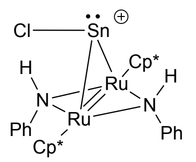
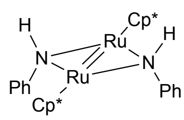
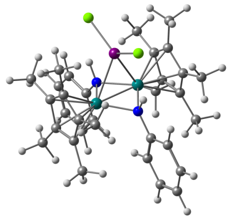
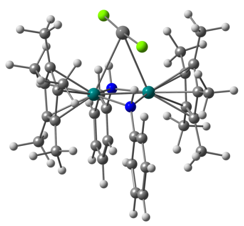
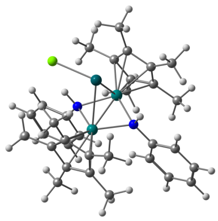
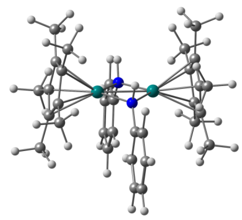
	2	**3**	**4**•(CH_2Cl_2)	**5**
formula	$C_{32}H_{42}Cl_2N_2Ru_2Zn$	$C_{33}H_{42}ClF_3N_2O_3Ru_2SSn$	$C_{35}H_{44}Cl_2F_3N_2O_3Ru_2SSn$	$C_{32}H_{42}Cl_2N_2PbRu_2$
M	793.09	960.04	1158.59	934.91
T/K	293(2)	173(2)	173(2)	293(2)
size (mm)	0.50 × 0.20 × 0.20	0.40 × 0.20 × 0.02	0.40 × 0.20 × 0.10	0.50 × 0.05 × 0.02
crystal system	orthorhombic	monoclinic	triclinic	orthorhombic
space group	*Pbca*	$P2_1/c$	*P*-1	*Pbca*
Z	8	8	2	8
a (Å)	17.836(4)	21.6780(5)	10.4804(7)	17.5750(6)
b (Å)	18.860(3)	15.5432(4)	10.7740(8)	18.5880(6)
c (Å)	19.709(4)	21.2981(5)	19.5872(14)	20.2407(8)
α (deg)	90.0000	90.0000	90.737(6)	90.0000
β (deg)	90.0000	94.863(7)	94.454(7)	90.0000
γ (deg)	90.0000	90.0000	104.508(7)	90.0000
V (Å^3)	6630(2)	7150.5(3)	2133.5(3)	6612.3(4)
D_{calc} (g/cm^3)	1.589	1.783	1.803	1.878
μ (mm^{-1})	1.802	1.711	1.573	6.176
reflns collected	56481	102766	19784	57606
unique reflns	7479	16257	9517	7513
GOF on F^2	1.016	1.030	1.315	1.000
R1 [$I > 2\sigma(I)$][a]	0.0256	0.0480	0.0604	0.0440
wR2 (all data)[b]	0.0666	0.1149	0.1718	0.0741

[a] $R1 = (\Sigma ||Fo| - |Fc||) / \Sigma |Fo|$, [b]$wR2 = [\{\Sigma (w(Fo^2 - Fc^2)^2)\} / \Sigma w(Fo^2)^2]^{1/2}$

Computational study

Geometry optimizations were performed with the B3PW91 hybrid functional[5] using the Gaussian 09 program[6] without any symmetry constraints in the gas phase. Ruthenium, zinc, tin, and lead atoms were described with the SDD effective core potentials and the associated basis sets,[7] while the 6-31G(d) basis set[8] was applied for all other atoms. The optimized geometries were checked by frequency calculations to confirm all positive frequencies. Natural bond orbital analyses were performed with NBO 6.0.19.[9] Molecular orbitals and natural bond orbitals were visualized by using the ChemCraft software.[10]

Table S2. Optimized geometries of **2**, **3**, **4** and **1'** with selected bond lengths (Å).[a]

<table>
<tr><td></td><td colspan="2"></td><td colspan="2"></td><td colspan="2"></td><td></td></tr>
<tr><td></td><td colspan="2">
2 (M = Zn)</td><td colspan="2">
3 (M = Pb)</td><td colspan="2">
4 (M = Sn)[a]</td><td>
1'</td></tr>
<tr><td></td><td>opt.</td><td>exp.</td><td>opt.</td><td>exp.</td><td>opt.</td><td>exp.</td><td>opt.</td></tr>
<tr><td>Ru1−Ru2</td><td>2.438</td><td>2.4201(5)</td><td>2.440</td><td>2.4309(6)</td><td>2.439</td><td>2.4195(6)</td><td>2.448</td></tr>
<tr><td>Ru1−M</td><td>2.619</td><td>2.5981(5)</td><td>2.950</td><td>2.8331(5)</td><td>2.784</td><td>2.7617(5)</td><td>----</td></tr>
<tr><td>Ru2−M</td><td>2.619</td><td>2.5975(5)</td><td>2.950</td><td>2.8468(5)</td><td>2.781</td><td>2.7722(6)</td><td>----</td></tr>
<tr><td>M−Cl1</td><td>2.256</td><td>2.2438(9)</td><td>2.884</td><td>2.867(2)</td><td>2.530</td><td>2.534(1)</td><td>----</td></tr>
<tr><td>M−Cl2</td><td>2.253</td><td>2.2246(9)</td><td>2.884</td><td>2.861(2)</td><td>----</td><td>----</td><td>----</td></tr>
<tr><td>Ru1−N1</td><td>2.068</td><td>2.058(1)</td><td>2.068</td><td>2.056(4)</td><td>2.082</td><td>2.060(4)</td><td>2.067</td></tr>
<tr><td>Ru1−N2</td><td>2.069</td><td>2.057(1)</td><td>2.069</td><td>2.071(4)</td><td>2.073</td><td>2.067(4)</td><td>2.066</td></tr>
<tr><td>Ru2−N1</td><td>2.069</td><td>2.064(1)</td><td>2.069</td><td>2.064(4)</td><td>2.083</td><td>2.060(4)</td><td>2.065</td></tr>
<tr><td>Ru2−N2</td><td>2.069</td><td>2.050(2)</td><td>2.068</td><td>2.055(4)</td><td>2.072</td><td>2.067(4)</td><td>2.064</td></tr>
</table>

[a] The OTf anion in **4** is omitted in the structral optimization.

Table S3. NBO analysis for $[(Cp^*Ru)_2(\mu\text{-}NHPh)_2ZnCl_2]$ (**2**).

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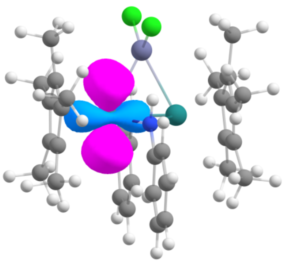
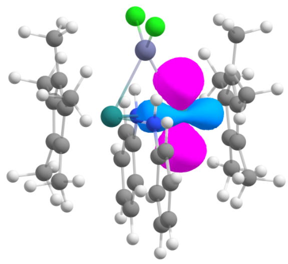
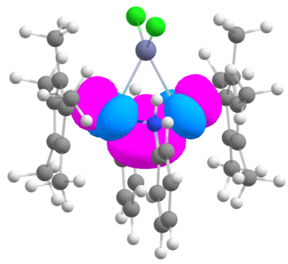
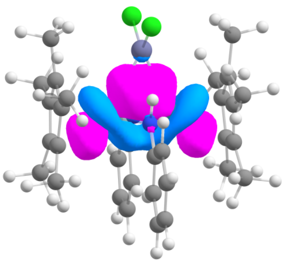
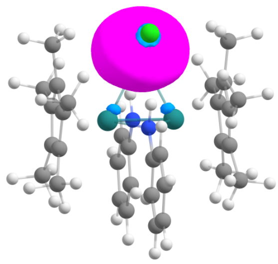
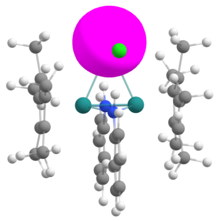
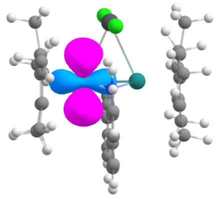
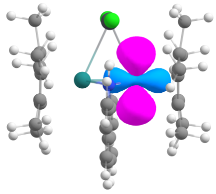
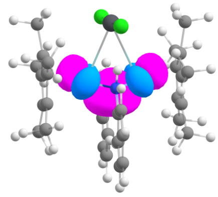
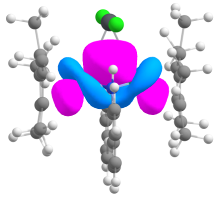
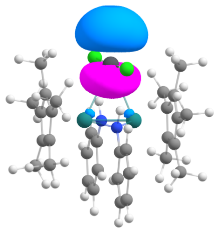
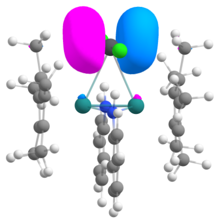
<tr><td></td><td></td><td colspan="2"></td></tr>
<tr><td>LP (Ru1)</td><td>LP (Ru2)</td><td colspan="2">BD (Ru1-Ru2)</td></tr>
<tr><td>occ. 1.89</td><td>occ. 1.89</td><td colspan="2">occ. 1.96</td></tr>
<tr><td>Ru1:
s (1.59%)
p (0.19%)
d (98.22%)</td><td>Ru2:
s (1.59%)
p (0.19%)
d (98.22%)</td><td>Ru1:
s (1.12 %)
p (0.04%)
d (98.84%)</td><td>Ru2:
s (1.11 %)
p (0.04%)
d (98.85%)</td></tr>
</table>

<table>
<tr><td colspan="2">NBO 79</td><td>NBO 170</td><td></td></tr>
<tr><td colspan="2"></td><td></td><td></td></tr>
<tr><td colspan="2">BD (Ru1-Ru2)</td><td>LV (Zn1)</td><td></td></tr>
<tr><td colspan="2">occ. 1.80</td><td>occ. 0.64</td><td></td></tr>
<tr><td>Ru1:
s (3.18%)
p (0.54%)
d (96.28%)</td><td>Ru2:
s (3.21%)
p (0.54%)
d (96.24%)</td><td>Zn1:
s (99.14%)
p (0.43%)
d (0.42%)</td><td></td></tr>
</table>

SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS		
Donor NBO	Acceptor NBO	*E*(2) kcal/mol
58, LP(Ru1)	170, LV (Zn1)	24.38
60, LP(Ru2)	170, LV (Zn1)	24.46
79, BD (Ru1-Ru2)	170, LV (Zn1)	77.20
68, LP (Cl)	177, BD* (N-H)	4.52
72, LP(Cl)	180, BD* (N-H)	3.97

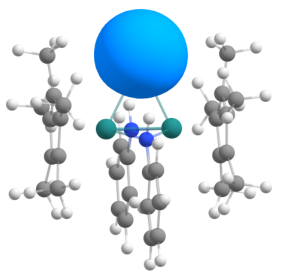
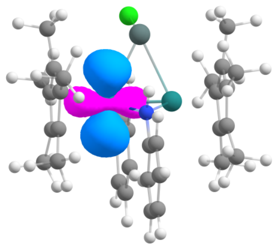
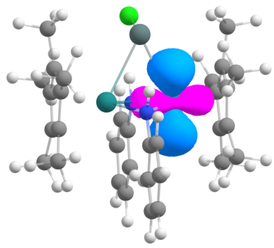
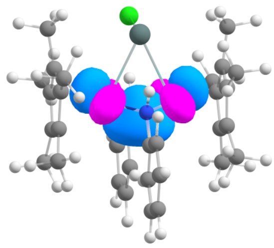
Table S4. NBO analysis for $[(Cp^*Ru)_2(\mu\text{-}NHPh)_2PbCl_2]$ (**3**).

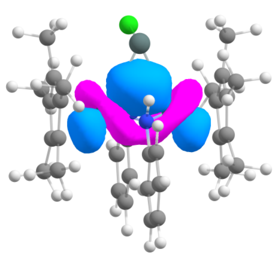
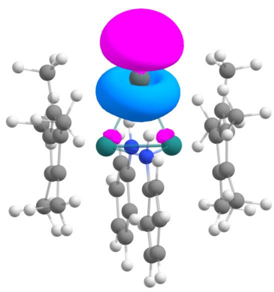
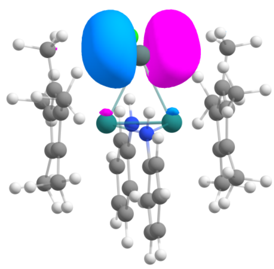
NBO 53	NBO 55	NBO 57	NBO 70	
				
LP (Pb1)	LP (Ru1)	LP (Ru2)	BD (Ru1-Ru2)	
occ. 1.97	occ. 1.83	occ. 1.83	occ. 1.95	
Pb1: s (97.16%) p (2.82%) d (0.02%)	Ru1: s (1.19%) p (0.11%) d (98.71%)	Ru2: s (1.19%) p (0.11%) d (98.71%)	Ru1: s (0.64%) p (0.04%) d (99.32%)	Ru2: s (0.64%) p (0.04%) d (99.32%)

NBO 71		NBO 160	NBO 162
			
BD (Ru1-Ru2)		LV (Pb1)	LV (Pb1)
occ. 1.75		occ. 0.51	occ. 0.31
Ru1: s(2.49%) p (0.29%) d (97.22%)	Ru2: s(2.49%) p (0.29%) d (97.22%)	Pb1: s (2.90%) p (97.09%) d (0.01%)	Pb1: s(0.00%) p (100.00%) d (0.00%)

SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS		
Donor NBO	Acceptor NBO	*E*(2) kcal/mol
55, LP(Ru1)	162, LV (Pb1)	37.78
57, LP(Ru2)	162, LV (Pb1)	37.77
55, LP(Ru1)	160, LV (Pb1)	11.74
57, LP(Ru2)	160, LV (Pb1)	11.75
71, BD (Ru1-Ru2)	160, LV (Pb1)	37.34
60, LP (Cl)	171, BD* (N-H)	13.10
64, LP (Cl)	174, BD* (N-H)	13.10

Table S5. NBO analysis for $[(Cp^*Ru)_2(\mu\text{-NHPh})_2SnCl]^+$ (**4**).

<table>
<tr><td>NBO 48</td><td>NBO 50</td><td>NBO 52</td><td colspan="2">NBO 62</td></tr>
<tr><td></td><td></td><td></td><td colspan="2"></td></tr>
<tr><td>LP (Sn1)</td><td>LP (Ru1)</td><td>LP (Ru2)</td><td colspan="2">BD (Ru1-Ru2)</td></tr>
<tr><td>occ. 1.96</td><td>occ. 1.80</td><td>occ. 1.80</td><td colspan="2">occ. 1.95</td></tr>
<tr><td>Sn1:
s (91.47%)
p (8.53%)</td><td>Ru1:
s (1.11%)
p (0.12%)
d (98.78%)</td><td>Ru2:
s (1.11%)
p (0.12%)
d (98.77%)</td><td>Ru1:
s (0.70%)
p (0.04%)
d (99.26%)</td><td>Ru2:
s (1.12%)
p (0.03%)
d (98.84%)</td></tr>
</table>

<table>
<tr><td colspan="2">NBO 63</td><td>NBO 151</td><td>NBO 152</td></tr>
<tr><td colspan="2"></td><td></td><td></td></tr>
<tr><td colspan="2">BD (Ru1-Ru2)</td><td>LV (Sn1)</td><td>LV (Sn1)</td></tr>
<tr><td colspan="2">occ. 1.75</td><td>occ. 0.60</td><td>occ. 0.29</td></tr>
<tr><td>Ru1:
s(2.27%)
p (0.18%)
d (97.55%)</td><td>Ru2:
s(1.75%)
p (0.15%)
d (98.10%)</td><td>Sn1:
s (7.22%)
p (92.78%)</td><td>Sn1:
s(0.00%)
p (100.00%)</td></tr>
</table>

<table>
<tr><td colspan="3">SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS</td></tr>
<tr><td>Donor NBO</td><td>Acceptor NBO</td><td>E(2) kcal/mol</td></tr>
<tr><td>50, LP(Ru1)</td><td>151, LV (Sn1)</td><td>21.14</td></tr>
<tr><td>50, LP(Ru1)</td><td>152, LV (Sn1)</td><td>40.39</td></tr>
<tr><td>52, LP(Ru2)</td><td>151, LV (Sn1)</td><td>21.17</td></tr>
<tr><td>52, LP(Ru2)</td><td>152, LV (Sn1)</td><td>41.12</td></tr>
<tr><td>63, BD (Ru1-Ru2)</td><td>151, LV (Sn1)</td><td>55.01</td></tr>
<tr><td>55, LP (Cl)</td><td>163, BD* (N-H)</td><td>10.90</td></tr>
</table>

Cartesian coordinates for $[(Cp^{*}Ru)_2(\mu\text{-}NHPh)_2ZnCl_2]$ (2)

44	0.036588000	1.218537000	0.020332000
44	-0.042304000	-1.217933000	0.018262000
30	0.017829000	0.001295000	-2.298598000
17	2.044290000	-0.058491000	-3.288264000
17	-1.974733000	0.061784000	-3.347677000
7	1.660468000	-0.053192000	0.175110000
7	-1.667742000	0.053685000	0.155595000
6	2.590943000	-0.084463000	1.243625000
6	2.179606000	-0.070820000	2.582336000
6	3.119906000	-0.099745000	3.606876000
6	4.486191000	-0.142725000	3.317994000
6	4.901954000	-0.157119000	1.987427000
6	3.963940000	-0.128792000	0.956630000
6	-2.607468000	0.082059000	1.216314000
6	-3.978170000	0.124477000	0.919065000
6	-4.923875000	0.149524000	1.943057000
6	-4.518028000	0.133829000	3.276629000
6	-3.153833000	0.092949000	3.575549000
6	-2.206119000	0.067334000	2.557993000
6	0.120222000	3.079708000	-1.290046000
6	-1.047006000	3.106973000	-0.458180000
6	-0.627416000	3.162712000	0.927353000
6	0.798259000	3.115619000	0.951233000
6	1.258383000	3.032282000	-0.420056000
6	0.147544000	3.239851000	-2.778215000
6	-2.455678000	3.211810000	-0.956103000
6	-1.524051000	3.406267000	2.099682000
6	1.669183000	3.308816000	2.151944000
6	2.688388000	3.047829000	-0.864956000
6	0.582360000	-3.163944000	0.951549000
6	1.056635000	-3.110493000	-0.416092000
6	-0.075515000	-3.079311000	-1.294649000
6	-1.248274000	-3.027400000	-0.471795000
6	-0.843006000	-3.110799000	0.917055000
6	1.429531000	-3.413208000	2.158856000
6	2.484189000	-3.219654000	-0.856034000
6	-0.044090000	-3.237478000	-2.782921000
6	-2.659335000	-3.041728000	-0.973956000

6	-1.763501000	-3.294466000	2.081963000
1	-0.751925000	2.832309000	-3.248189000
1	0.202500000	4.308878000	-3.031498000
1	1.013359000	2.745989000	-3.228097000
1	-2.704725000	4.257729000	-1.182935000
1	-2.598762000	2.625431000	-1.869063000
1	-3.174395000	2.857563000	-0.211208000
1	3.027694000	4.080777000	-1.024630000
1	2.821706000	2.500389000	-1.802881000
1	3.347753000	2.597899000	-0.116621000
1	1.913408000	4.374019000	2.272655000
1	1.174711000	2.977514000	3.069414000
1	2.611882000	2.762132000	2.069710000
1	-1.698825000	4.484583000	2.223839000
1	-1.086809000	3.032298000	3.029625000
1	-2.497915000	2.925923000	1.977537000
1	-1.143606000	0.033512000	2.778097000
1	-2.826002000	0.080596000	4.612337000
1	-5.254503000	0.153121000	4.075245000
1	-5.981307000	0.181352000	1.693067000
1	-4.298790000	0.136700000	-0.120840000
1	-2.171656000	0.069718000	-0.735053000
1	2.171899000	-0.067642000	-0.711609000
1	1.115684000	-0.035548000	2.795193000
1	2.784414000	-0.088357000	4.641200000
1	5.216655000	-0.164634000	4.122051000
1	5.961143000	-0.190472000	1.745204000
1	4.291799000	-0.140054000	-0.080972000
1	3.172753000	-2.865622000	-0.083207000
1	2.666526000	-2.636372000	-1.763938000
1	2.739104000	-4.266768000	-1.070575000
1	0.865177000	-2.814845000	-3.219458000
1	-0.073753000	-4.306649000	-3.039842000
1	-0.900768000	-2.755988000	-3.262835000
1	-3.348371000	-2.594922000	-0.250789000
1	-2.756221000	-2.490815000	-1.914359000
1	-2.715382000	-2.777169000	1.937894000
1	-1.324277000	-2.921574000	3.011380000
1	-1.984619000	-4.362211000	2.222681000

1	0.945104000	-3.059886000	3.073497000
1	1.613570000	-4.490855000	2.275422000
1	2.401053000	-2.917984000	2.088017000
1	-2.991425000	-4.074285000	-1.150322000

Cartesian coordinates for [(Cp*Ru)$_2$(μ-NHPh)$_2$PbCl$_2$] (3)

82	-0.000501000	-2.425320000	-0.000135000
44	0.048647000	0.260215000	1.219091000
44	-0.048515000	0.260365000	-1.219026000
17	2.882705000	-2.496430000	0.012539000
17	-2.883723000	-2.495231000	-0.012962000
7	1.657862000	0.449691000	-0.066706000
7	-1.657663000	0.450316000	0.066789000
6	2.553771000	1.545895000	-0.116311000
6	3.931198000	1.285327000	-0.208142000
6	4.843135000	2.337046000	-0.270614000
6	4.399990000	3.659535000	-0.240872000
6	3.031451000	3.920862000	-0.145992000
6	2.115203000	2.875512000	-0.084527000
6	-2.553231000	1.546798000	0.116504000
6	-3.930750000	1.286633000	0.208158000
6	-4.842373000	2.338612000	0.270771000
6	-4.398825000	3.660973000	0.241363000
6	-3.030198000	3.921902000	0.146669000
6	-2.114255000	2.876286000	0.085052000
6	0.285430000	-0.964429000	3.144223000
6	1.334667000	0.005662000	3.055715000
6	0.742292000	1.324063000	3.089552000
6	-0.674185000	1.161371000	3.150948000
6	-0.963220000	-0.255854000	3.150496000
6	-0.285850000	-0.963799000	-3.144454000
6	0.963164000	-0.255876000	-3.150515000
6	0.674843000	1.161504000	-3.150727000
6	-0.741546000	1.324910000	-3.089373000
6	-1.334599000	0.006798000	-3.055769000
6	2.317080000	-0.871768000	-3.323370000
1	2.493715000	-1.112832000	-4.380940000
1	3.108336000	-0.188306000	-3.003639000

1	2.431599000	-1.786895000	-2.735522000
6	-0.468844000	-2.431787000	-3.368340000
1	-1.353932000	-2.822587000	-2.854622000
1	-0.604876000	-2.625711000	-4.442067000
1	0.407702000	-3.009513000	-3.053413000
6	-2.800261000	-0.295856000	-3.084488000
1	-3.386972000	0.521595000	-2.656169000
1	-3.135792000	-0.436806000	-4.121527000
1	-3.036476000	-1.202522000	-2.519438000
6	-1.485474000	2.615271000	-3.223569000
1	-1.684126000	2.827172000	-4.283874000
1	-2.446283000	2.590025000	-2.704738000
1	-0.914647000	3.456345000	-2.819395000
6	1.676066000	2.251068000	-3.367673000
1	1.857993000	2.376442000	-4.444440000
1	1.325725000	3.209393000	-2.976388000
1	2.635715000	2.032822000	-2.892886000
6	2.800174000	-0.297775000	3.084302000
1	3.135656000	-0.439251000	4.121286000
1	3.035894000	-1.204392000	2.518966000
1	3.387323000	0.519496000	2.656243000
6	0.467693000	-2.432542000	3.367872000
1	0.603553000	-2.626704000	4.441574000
1	-0.409112000	-3.009788000	3.052774000
1	1.352623000	-2.823669000	2.854126000
6	1.486916000	2.614005000	3.223959000
1	1.685860000	2.825517000	4.284285000
1	2.447618000	2.588383000	2.704944000
1	0.916465000	3.455489000	2.820094000
6	-1.674815000	2.251441000	3.368074000
1	-2.634642000	2.033723000	2.893409000
1	-1.856530000	2.376889000	4.444869000
1	-1.324012000	3.209588000	2.976768000
6	-2.317454000	-0.871096000	3.323231000
1	-2.432420000	-1.786132000	2.735323000
1	-2.494264000	-1.112159000	4.380774000
1	-3.108362000	-0.187222000	3.003521000
1	4.272816000	0.252458000	-0.227924000
1	5.905581000	2.118272000	-0.341793000

1	5.112317000	4.478703000	-0.289258000
1	2.675275000	4.948028000	-0.119098000
1	1.050290000	3.069682000	-0.008515000
1	2.209507000	-0.422543000	-0.076391000
1	-2.209597000	-0.421731000	0.076370000
1	-4.272682000	0.253862000	0.227705000
1	-5.904891000	2.120136000	0.341805000
1	-5.110899000	4.480352000	0.289871000
1	-2.673705000	4.948965000	0.120047000
1	-1.049279000	3.070183000	0.009176000

Cartesian coordinates for [(Cp*Ru)$_2$(μ-NHPh)$_2$SnCl]$^+$ (4)

50	0.884473000	-0.077472000	-2.410260000
44	-0.180865000	-1.207506000	-0.099575000
44	0.042429000	1.221057000	-0.099190000
17	3.320842000	-0.300888000	-1.767847000
7	1.344630000	-0.122875000	0.790627000
7	-1.678450000	0.154409000	-0.587252000
6	1.704081000	-0.156161000	2.163497000
6	3.059479000	-0.295195000	2.503950000
6	3.447984000	-0.334426000	3.841254000
6	2.493933000	-0.235429000	4.854263000
6	1.145653000	-0.095859000	4.518460000
6	0.751987000	-0.056325000	3.184454000
6	-2.937128000	0.267075000	0.066574000
6	-4.102100000	0.365147000	-0.708175000
6	-5.349533000	0.474319000	-0.096673000
6	-5.450252000	0.488006000	1.294159000
6	-4.291808000	0.391672000	2.067549000
6	-3.044100000	0.282539000	1.461381000
1	-2.140947000	0.207402000	2.057356000
6	-0.228230000	-3.120607000	1.115472000
6	0.860859000	-3.192538000	0.166451000
6	0.311135000	-3.187844000	-1.156379000
6	-1.108838000	-3.014018000	-1.033907000
6	-1.443162000	-3.011488000	0.375491000
6	0.282936000	3.123280000	1.120662000
6	1.412242000	2.986305000	0.228132000

6	0.938910000	3.070432000	-1.121262000
6	-0.494346000	3.158313000	-1.071390000
6	-0.892357000	3.227929000	0.318690000
6	2.300473000	-3.418272000	0.505454000
1	2.560808000	-2.986908000	1.475553000
1	2.505628000	-4.495819000	0.559092000
1	2.967074000	-2.987554000	-0.246703000
6	-0.106491000	-3.305071000	2.593522000
1	-0.121314000	-4.377030000	2.834155000
1	0.826200000	-2.891958000	2.983816000
1	-0.932732000	-2.835106000	3.133286000
6	1.061336000	-3.476415000	-2.417181000
1	1.091235000	-4.562449000	-2.581445000
1	0.582395000	-3.038581000	-3.299998000
1	2.096516000	-3.124705000	-2.374629000
6	-2.092586000	-3.038752000	-2.162984000
1	-2.375971000	-4.073017000	-2.398960000
1	-3.010870000	-2.500141000	-1.911419000
1	-1.680109000	-2.598572000	-3.076961000
6	-2.825682000	-3.071140000	0.940631000
1	-3.547561000	-2.521540000	0.332018000
1	-3.156176000	-4.117971000	0.983028000
1	-2.871297000	-2.668287000	1.955000000
6	-1.398931000	3.353259000	-2.248675000
1	-1.478920000	4.419740000	-2.497583000
1	-1.025957000	2.838302000	-3.140036000
1	-2.410946000	2.990490000	-2.046573000
6	1.789635000	3.214837000	-2.342455000
1	2.007262000	4.278970000	-2.508389000
1	2.747152000	2.694837000	-2.247579000
1	1.288604000	2.853588000	-3.248056000
6	-2.267905000	3.540363000	0.813465000
1	-2.441074000	3.149107000	1.818608000
1	-2.400012000	4.630192000	0.852393000
1	-3.046682000	3.137286000	0.161682000
6	0.358225000	3.298678000	2.603190000
1	0.533486000	4.356788000	2.841573000
1	-0.571277000	3.000911000	3.095758000
1	1.172581000	2.721186000	3.046217000

6	2.849744000	2.941672000	0.640362000
1	3.252409000	3.961663000	0.699371000
1	2.974779000	2.481637000	1.623959000
1	3.459554000	2.381961000	-0.074478000
1	-4.032204000	0.355548000	-1.795140000
1	-6.242563000	0.548999000	-0.710855000
1	-6.421881000	0.573170000	1.771585000
1	-4.361578000	0.401775000	3.152107000
1	-1.863120000	0.169661000	-1.589624000
1	2.200180000	-0.202321000	0.231238000
1	-0.293365000	0.052680000	2.917108000
1	0.396422000	-0.017577000	5.301824000
1	2.797396000	-0.266107000	5.896612000
1	4.500066000	-0.442454000	4.089686000
1	3.805760000	-0.371828000	1.715979000

Cartesian coordinates for [Cp*Ru(μ-NHPh)]$_2$ (1)

7	1.286382000	-0.105638000	-0.922704000
6	2.684914000	-0.209642000	-0.839387000
6	3.312235000	-0.308552000	0.412451000
6	4.697223000	-0.407083000	0.510237000
6	5.494852000	-0.410874000	-0.636314000
6	4.880805000	-0.315397000	-1.884500000
6	3.494712000	-0.215758000	-1.986838000
6	0.323469000	3.612938000	-0.540385000
6	1.459833000	3.201615000	0.253060000
6	0.950400000	2.677481000	1.479996000
6	0.499278000	-2.818062000	1.472403000
6	0.882050000	-3.424225000	0.237856000
6	-0.323270000	-3.613109000	-0.539169000
6	-0.881940000	3.424429000	0.236597000
6	-0.499343000	2.818780000	1.471441000
6	-0.950486000	-2.676871000	1.480760000
6	-1.459749000	-3.201569000	0.253989000
7	-1.286469000	0.105455000	-0.922677000
6	-2.684997000	0.209317000	-0.839145000
6	-3.312103000	0.308878000	0.412748000
6	-4.697085000	0.407254000	0.510741000
6	-5.494938000	0.410224000	-0.635658000

6	-4.881112000	0.314094000	-1.883902000
6	-3.495021000	0.214616000	-1.986440000
6	0.394148000	4.248202000	-1.892874000
1	0.501688000	5.339145000	-1.804426000
1	1.249878000	3.877567000	-2.465746000
1	-0.510554000	4.051511000	-2.476623000
6	-2.263765000	3.837952000	-0.161171000
1	-3.018806000	3.150128000	0.230889000
1	-2.494988000	4.845522000	0.213020000
1	-2.381149000	3.857583000	-1.249255000
6	-1.393863000	2.539052000	2.636780000
1	-1.358562000	3.370236000	3.356152000
1	-2.434494000	2.418910000	2.324125000
1	-1.093580000	1.631832000	3.171558000
6	1.751429000	2.210996000	2.653022000
1	2.759990000	1.908891000	2.358516000
1	1.848870000	3.013133000	3.398931000
1	1.274923000	1.358055000	3.147198000
6	2.897387000	3.336490000	-0.136821000
1	3.294031000	4.320173000	0.152268000
1	3.516619000	2.569173000	0.336214000
1	3.029353000	3.230285000	-1.218188000
6	2.263921000	-3.837869000	-0.159608000
1	3.018923000	-3.149931000	0.232327000
1	2.495096000	-4.845326000	0.214919000
1	2.381435000	-3.857830000	-1.247672000
6	-0.393788000	-4.248850000	-1.891438000
1	-0.501331000	-5.339765000	-1.802627000
1	-1.249464000	-3.878421000	-2.464528000
1	0.510979000	-4.052351000	-2.475150000
6	-2.897231000	-3.336747000	-0.136035000
1	-3.293539000	-4.320709000	0.152570000
1	-3.516748000	-2.569893000	0.337355000
1	-3.029195000	-3.230074000	-1.217358000
6	-1.751629000	-2.210101000	2.653610000
1	-2.760102000	-1.907880000	2.358936000
1	-1.849272000	-3.012118000	3.399619000
1	-1.275058000	-1.357151000	3.147715000
6	1.393653000	-2.537681000	2.637699000

1	1.358147000	-3.368382000	3.357620000
1	2.434344000	-2.417863000	2.325121000
1	1.093369000	-1.630073000	3.171807000
1	5.158999000	-0.482925000	1.492590000
1	6.575813000	-0.487437000	-0.557111000
1	5.483325000	-0.317405000	-2.790087000
1	2.685016000	-0.309382000	1.298166000
1	3.029017000	-0.140611000	-2.969027000
1	1.035979000	-0.078776000	-1.916742000
1	-1.036267000	0.078252000	-1.916751000
1	-3.029502000	0.138944000	-2.968673000
1	-5.483802000	0.315458000	-2.789378000
1	-6.575896000	0.486664000	-0.556290000
1	-5.158686000	0.483610000	1.493136000
1	-2.684721000	0.310295000	1.298339000
44	-0.123542000	-1.518182000	-0.160573000
44	0.123555000	1.518197000	-0.160973000

Cartesian coordinates for [Cp*Ru(μ-NHPh)]$_2$ (1')

44	1.229774000	0.016577000	-0.410033000
44	-1.217552000	-0.014238000	-0.444488000
7	0.027925000	-1.661056000	-0.368889000
7	-0.014294000	1.664330000	-0.369025000
6	0.028586000	-2.631961000	0.660989000
6	0.119380000	-3.995750000	0.345945000
6	0.117638000	-4.961494000	1.352234000
6	0.023153000	-4.582907000	2.689537000
6	-0.068219000	-3.224728000	3.008596000
6	-0.064644000	-2.258366000	2.009144000
6	-0.039486000	2.635819000	0.660110000
6	-0.001714000	4.001715000	0.342909000
6	-0.030411000	4.968340000	1.347690000
6	-0.099097000	4.588800000	2.686344000
6	-0.137511000	3.228702000	3.007814000
6	-0.107470000	2.261342000	2.009479000
6	3.040119000	0.102363000	-1.817566000
6	3.074433000	-1.089530000	-1.026194000
6	3.219249000	-0.726534000	0.371419000
6	3.222926000	0.695474000	0.449106000

6	3.070604000	1.201820000	-0.899247000
6	3.037558000	0.186011000	-3.311144000
6	3.109437000	-2.487726000	-1.562241000
6	3.457409000	-1.678193000	1.501373000
6	3.467114000	1.520563000	1.673057000
6	3.100418000	2.649357000	-1.282381000
6	-2.956452000	0.682516000	-1.655404000
6	-3.170724000	1.104468000	-0.285624000
6	-3.331208000	-0.051913000	0.540768000
6	-3.137668000	-1.192006000	-0.301530000
6	-2.936162000	-0.746407000	-1.665193000
6	-2.889047000	1.578089000	-2.853010000
6	-3.374706000	2.517984000	0.163993000
6	-3.702803000	-0.068572000	1.989268000
6	-3.298034000	-2.616737000	0.129562000
6	-2.841643000	-1.624140000	-2.874041000
1	-3.837624000	-1.867730000	-3.272211000
1	-2.273343000	-1.140817000	-3.675256000
1	-2.347076000	-2.574492000	-2.645984000
1	-2.307343000	1.122348000	-3.660770000
1	-2.423277000	2.540147000	-2.613652000
1	-3.892295000	1.796443000	-3.247481000
1	-4.442935000	2.775717000	0.139582000
1	-2.851226000	3.231845000	-0.478199000
1	-3.015770000	2.678550000	1.184934000
1	-4.794692000	-0.110135000	2.121804000
1	-3.345852000	0.828399000	2.504942000
1	-3.278433000	-0.937313000	2.502565000
1	-2.741741000	-3.305099000	-0.513153000
1	-4.356287000	-2.911020000	0.088333000
1	-2.947122000	-2.775518000	1.153448000
1	4.061515000	0.230588000	-3.712284000
1	2.509711000	1.077861000	-3.663748000
1	2.546786000	-0.682172000	-3.762057000
1	2.569812000	2.829306000	-2.224019000
1	4.134387000	2.995035000	-1.421211000
1	2.643677000	3.281042000	-0.514463000
1	2.901795000	2.456858000	1.653697000
1	4.532342000	1.778925000	1.768277000

1	3.175827000	0.984038000	2.581380000
1	4.528049000	-1.910336000	1.600812000
1	2.927046000	-2.623898000	1.356770000
1	3.118633000	-1.260945000	2.454440000
1	2.673337000	-3.202203000	-0.856800000
1	4.142976000	-2.807744000	-1.755077000
1	2.562083000	-2.571287000	-2.507955000
1	0.047683000	4.307186000	-0.701391000
1	-0.000950000	6.021433000	1.078279000
1	-0.122029000	5.340378000	3.470880000
1	-0.190066000	2.919318000	4.049175000
1	-0.135875000	1.200200000	2.239192000
1	0.187144000	-4.300517000	-0.697562000
1	0.187652000	-6.013210000	1.084958000
1	0.020621000	-5.333836000	3.475024000
1	-0.141546000	-2.916395000	4.049027000
1	-0.133745000	-1.198612000	2.236301000
1	0.062483000	-2.135211000	-1.270182000
1	0.006323000	2.138642000	-1.270582000

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