Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Synthesis and Characterisation of Ruthenium Dihydrogen Complexes and their Reactivity towards B-H Bonds

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T1 measurements of complex 4-6

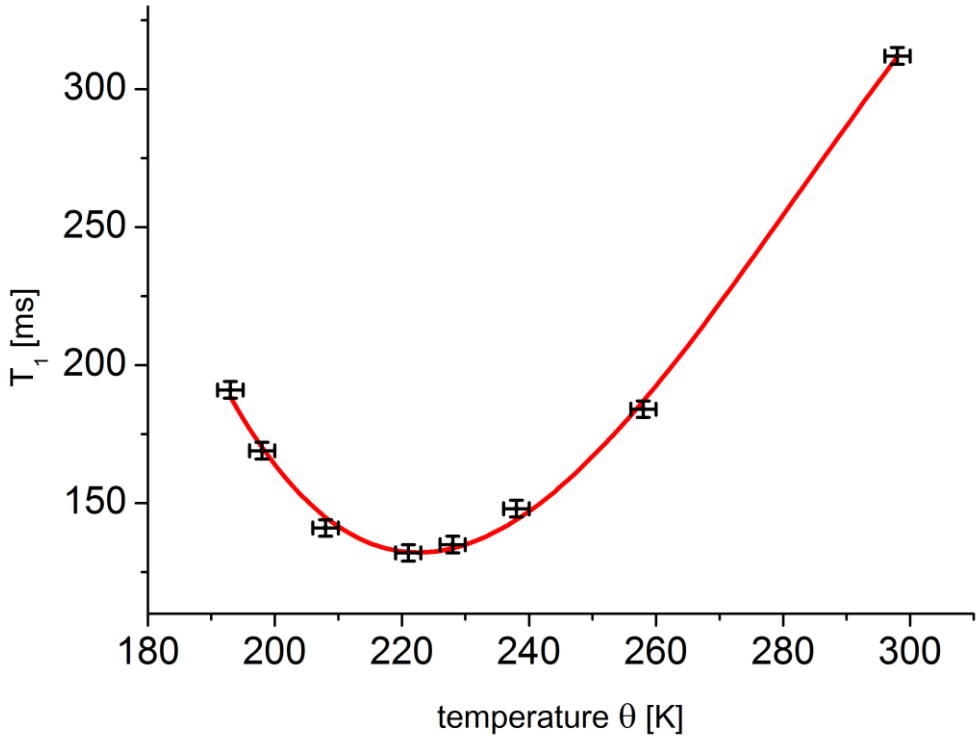

Figure S1 T_1 values of [Ru(H_2)H_2(PNP)] **4** as a function of the temperature Θ [K] at 500 MHz.

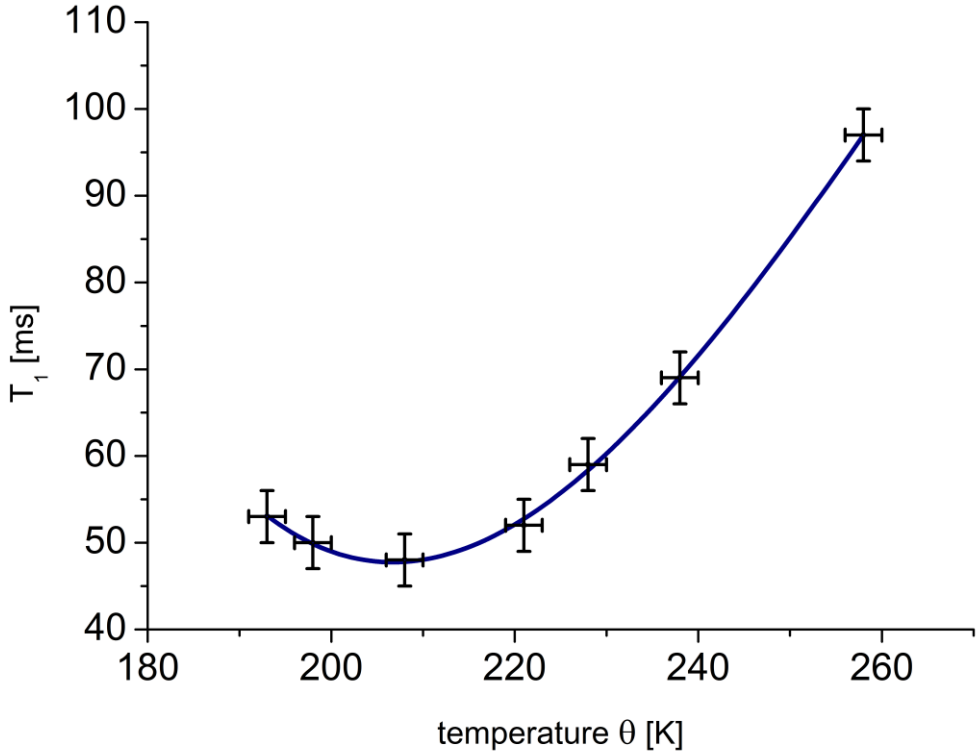

Figure S2 T_1 values of [Ru(H_2)H(PNP)] **5** as a function of the temperature Θ [K] at 500 MHz.

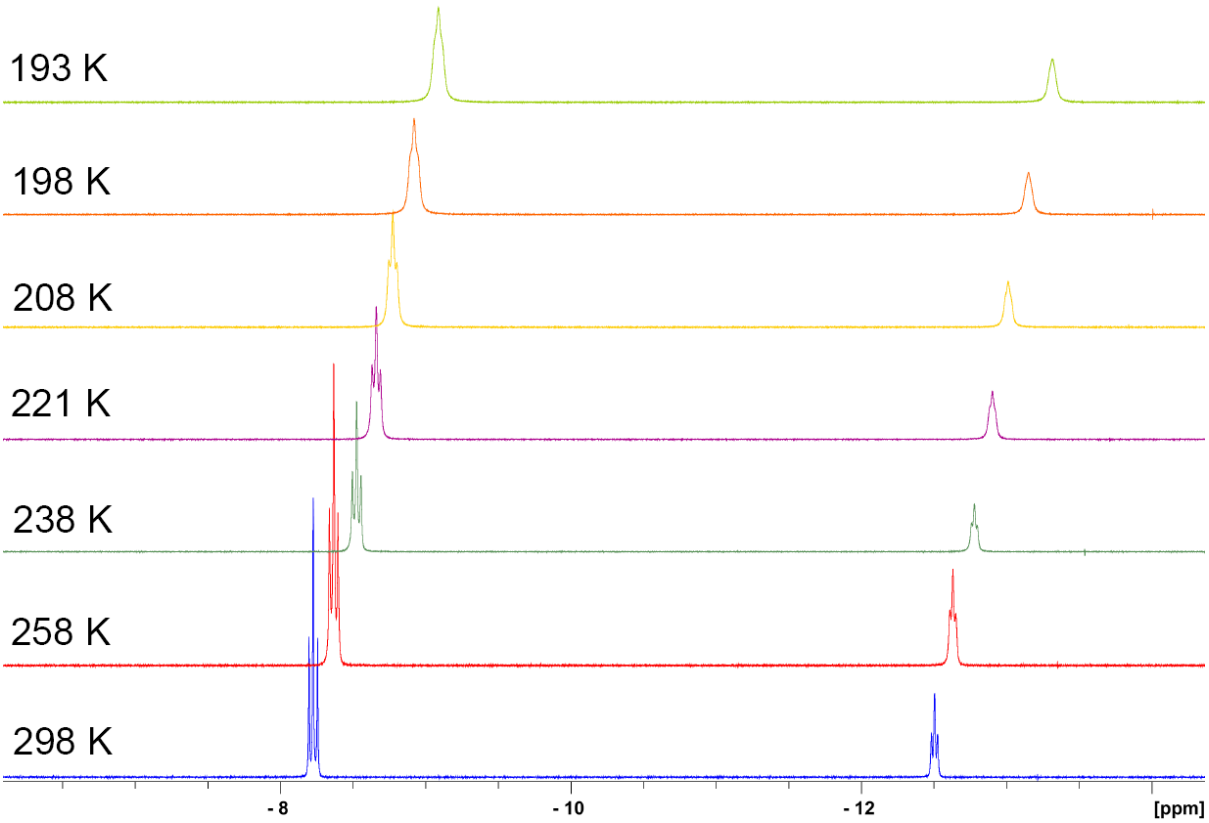

Figure S3 Hydride signals of complex **4** (-8.26 ppm) and **5** (-12.44 ppm) during T1-measurements between 298 K – 193 K.

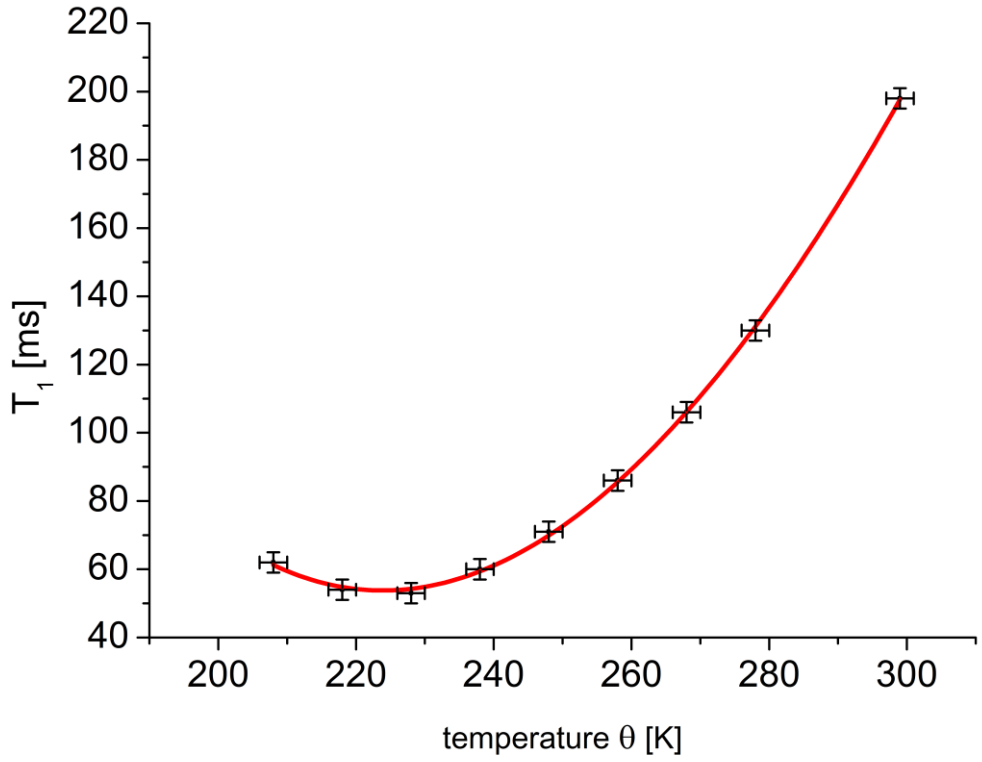

Figure S4 T_1 values of [Ru(H_2)H(MePNP)] **6** as a function of the temperature Θ [K] at 500 MHz.

IR data of complexes 4-7

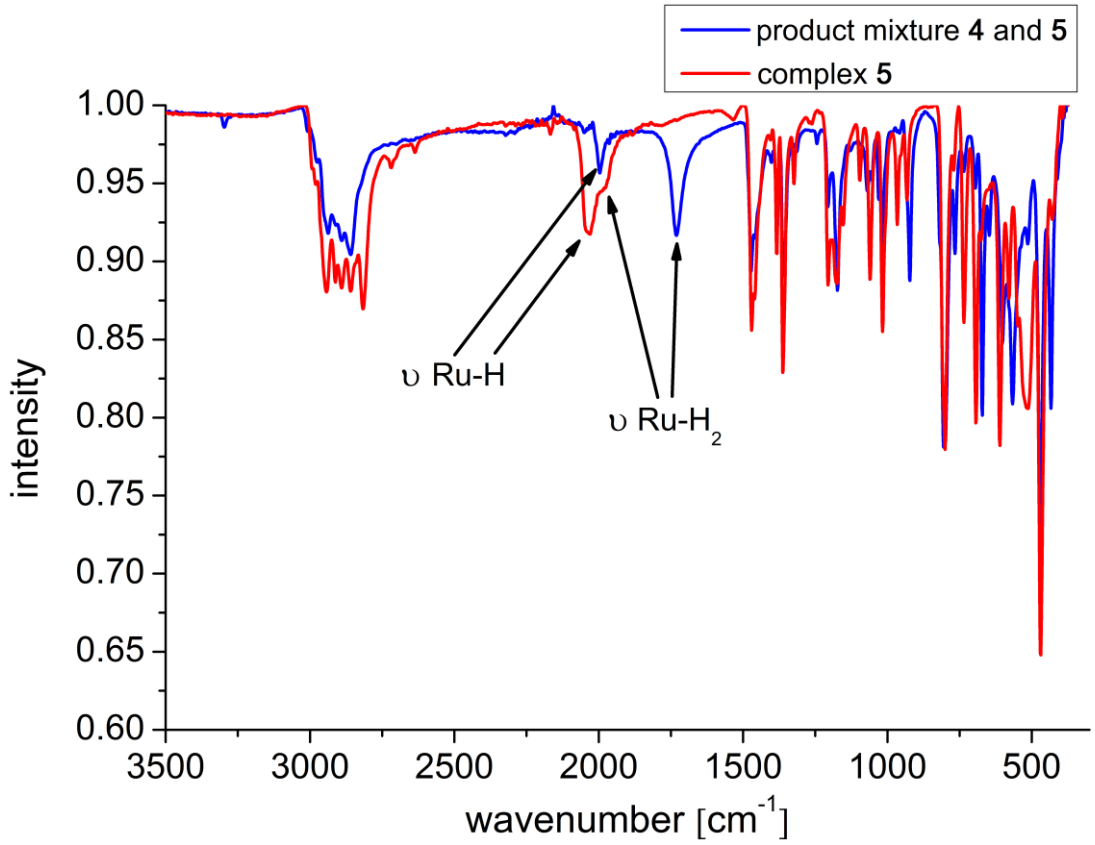

Figure S5 IR spectra of the product mixture **4** and **5** (blue) and [Ru(H_2)H(PNP)] **5** (red).

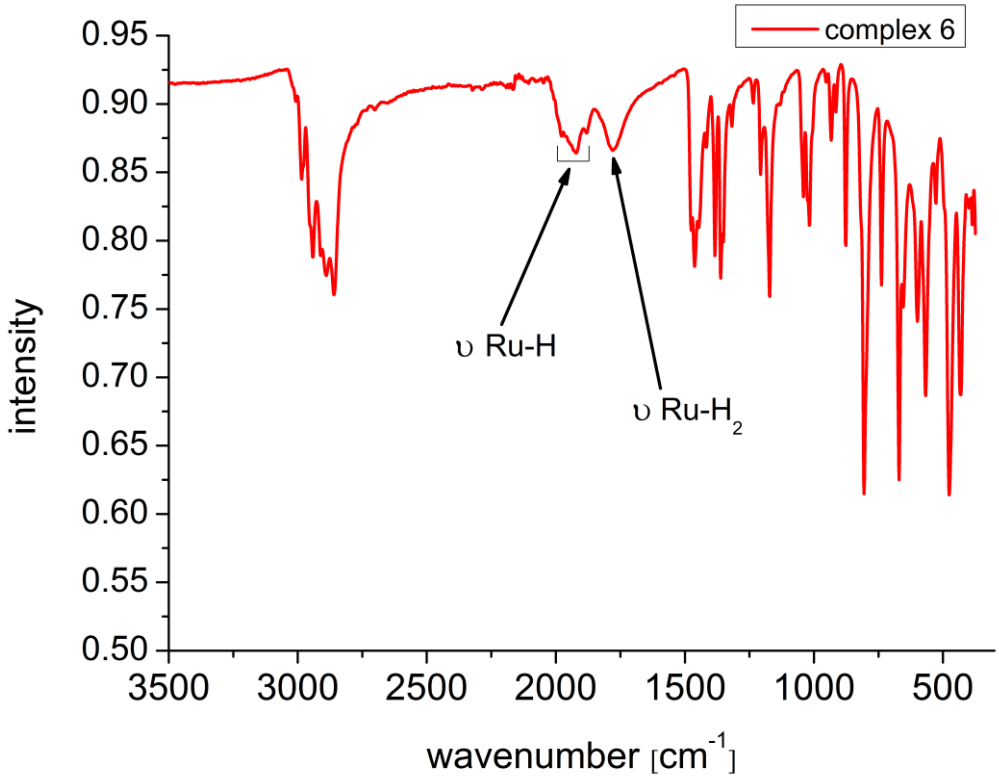

Figure S6 IR spectrum of [Ru(H_2)H_2(Me-PNP)] **6** (red).

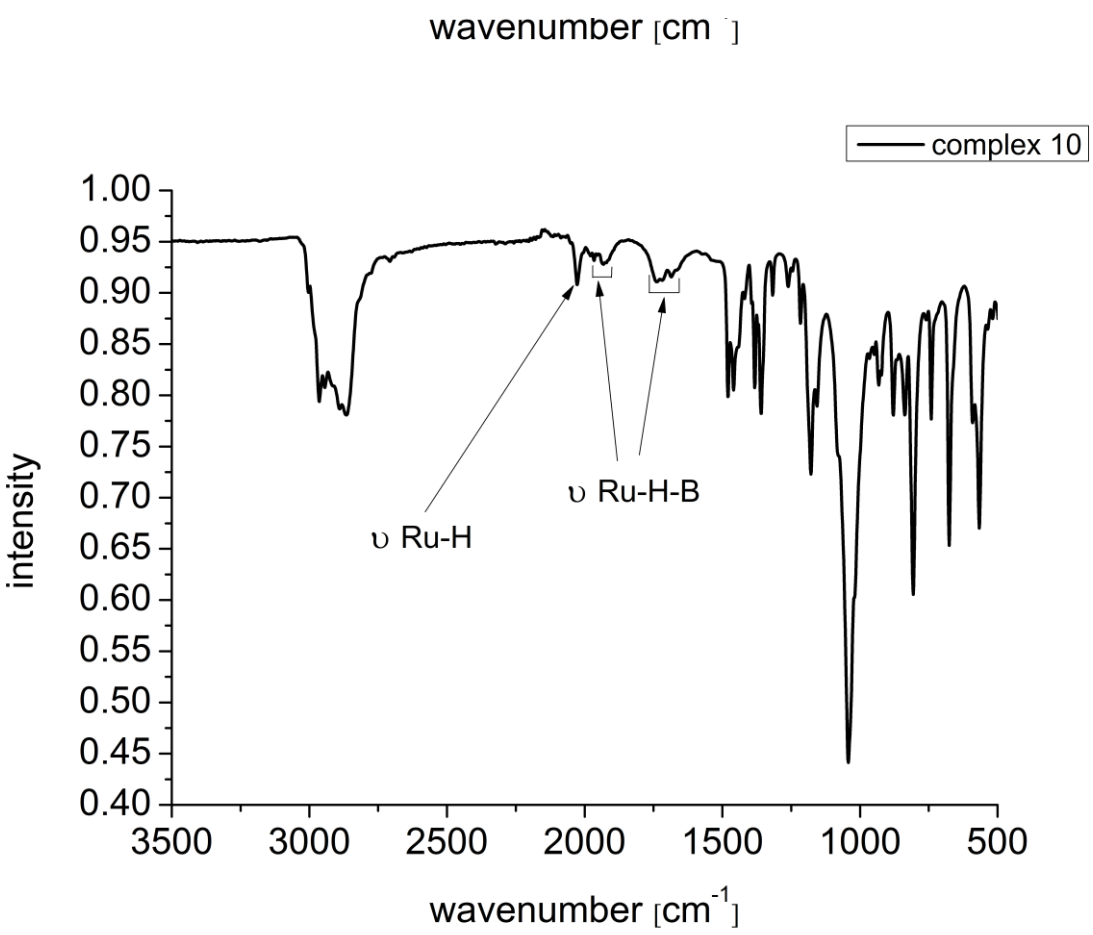

Figure S7 IR spectrum of [RuH_2(HBPin)(Me-PNP)] **10**.

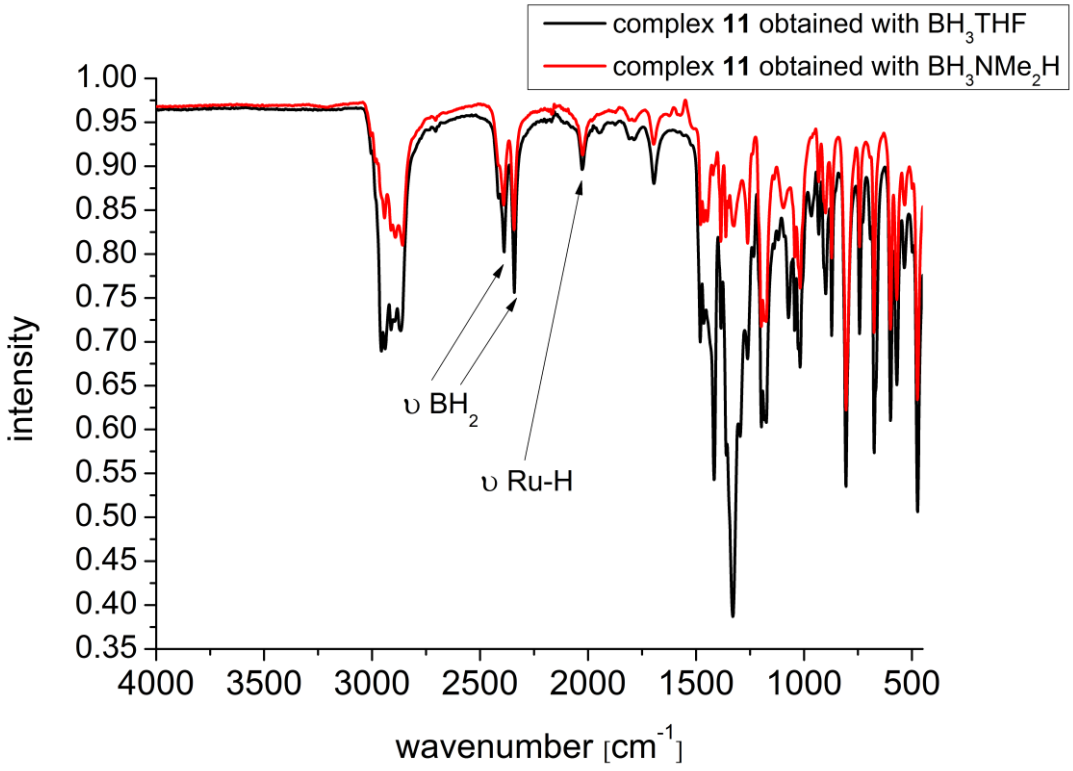

Figure S8 IR spectra of complex **11**. Vibrational bands are identical beside the THF traces independent from the different synthetic route with BH_3THF (black) or BH_3NMe_2H (red).

LIFDI-MS DATA of complexes 5, 6, 10, 11

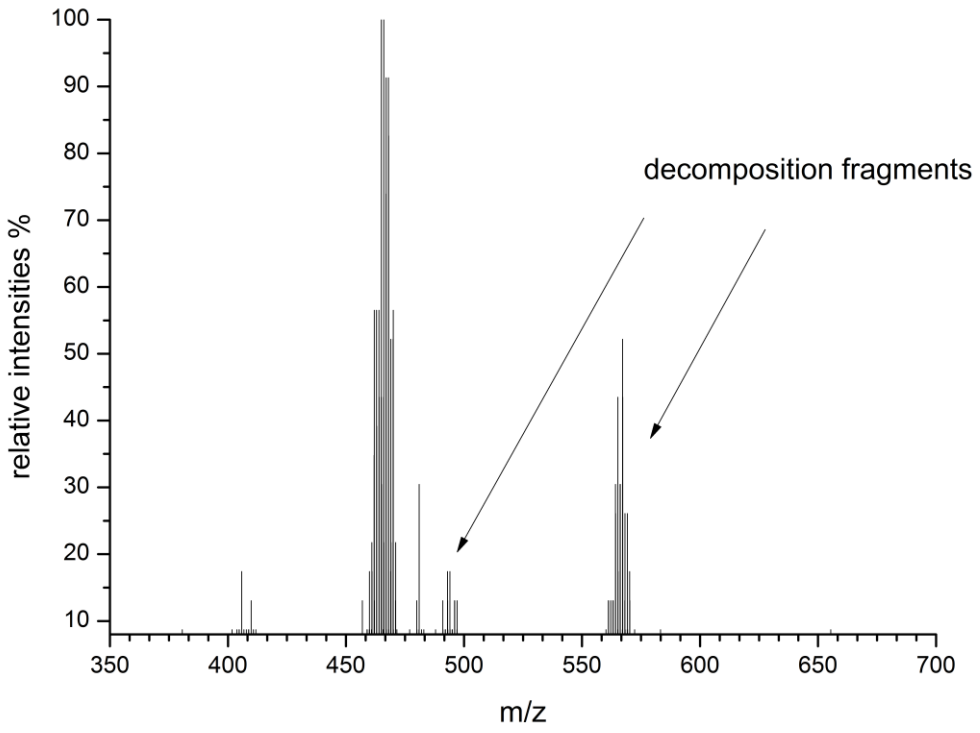

Figure S9 LIFDI-MS of [Ru(H_2)H(PNP)] **5** in toluene. Retention time (RT) at 3.14 min of 5.00 min. Decomposition of the analysed complexes begins when starting extensive heating of the filament during MS analysis.

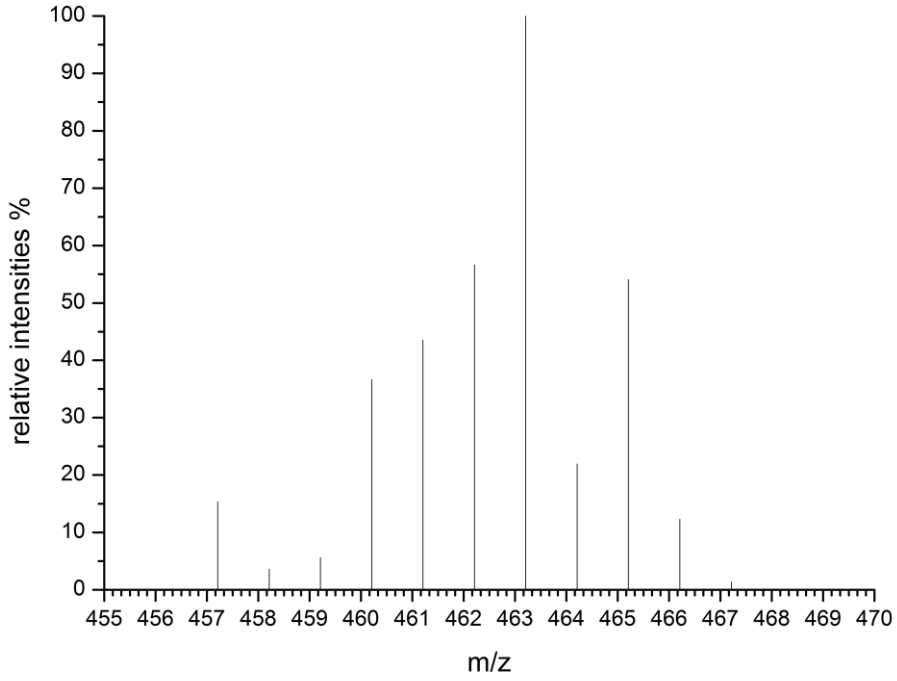

Figure S10 Simulated isotope pattern of [RuH(PNP)] 463.

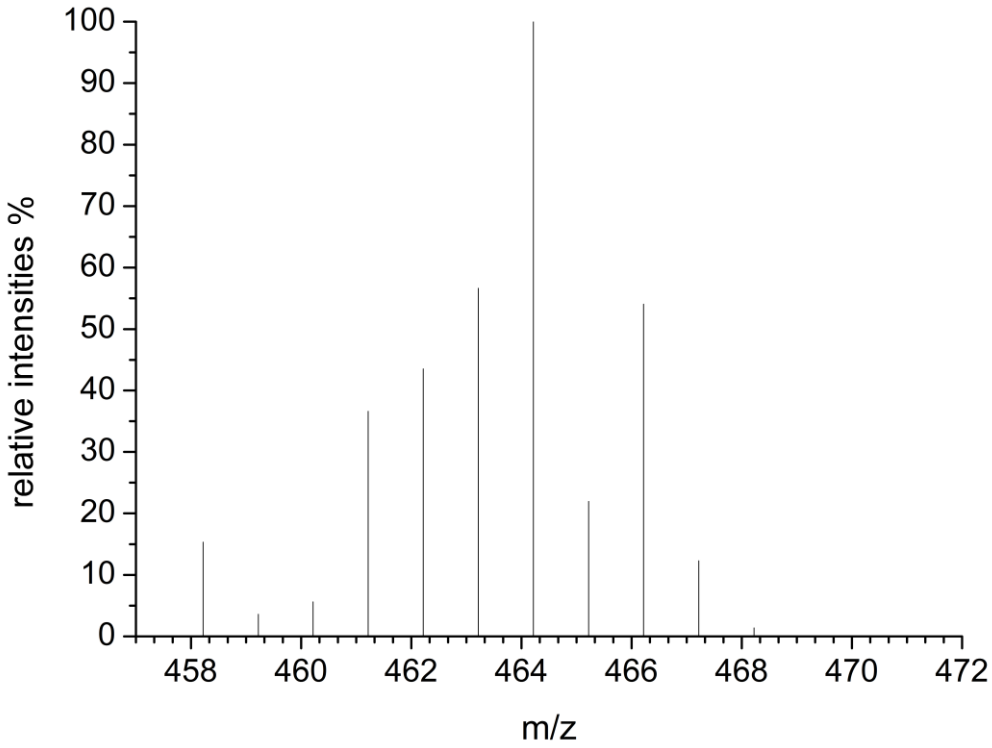

Figure S11 Simulated isotope pattern of [RuH_2(PNP)] 464.

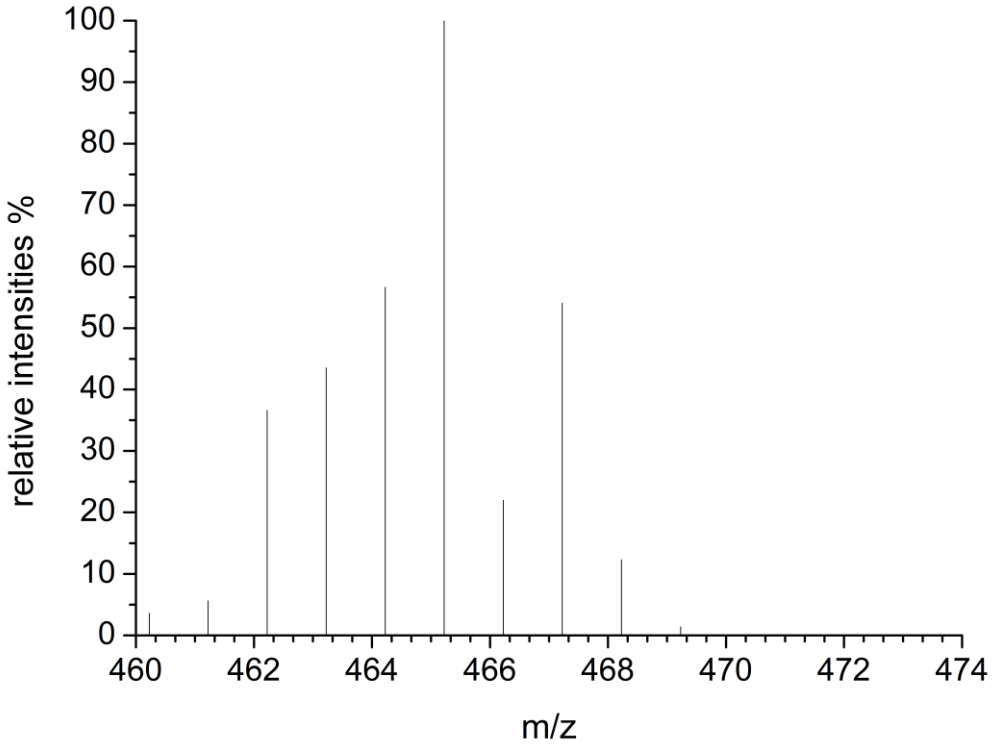

Figure S12 Simulated isotope pattern of [Ru(H_2)H(PNP)] 465.

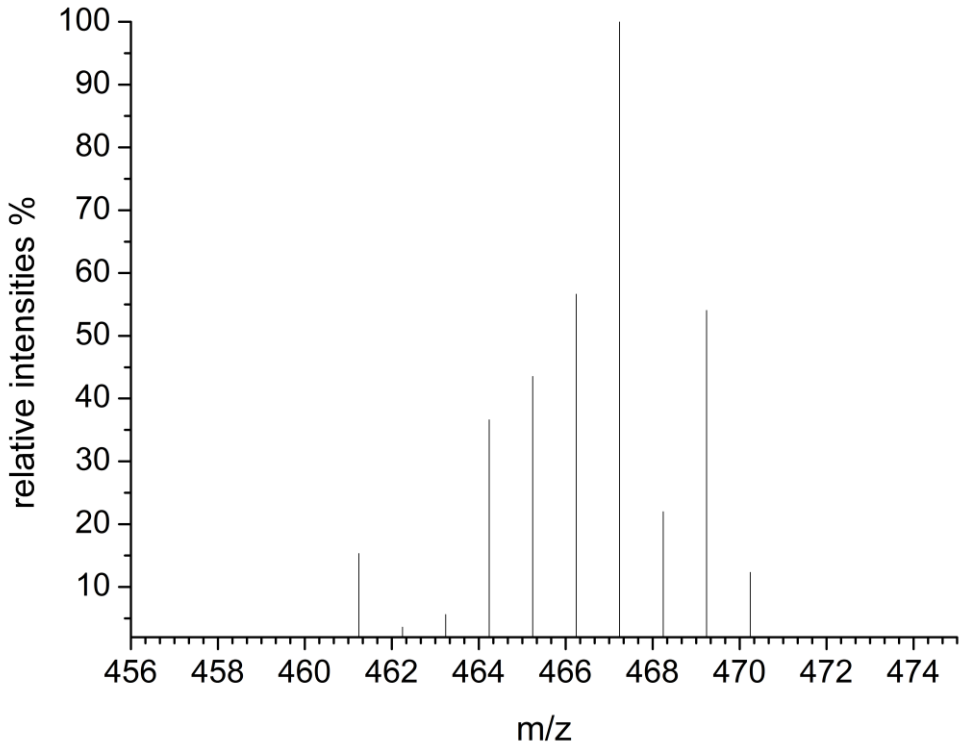

Figure S13 Simulated isotope pattern of [Ru(H_2)H_2(HPNP)] 467.

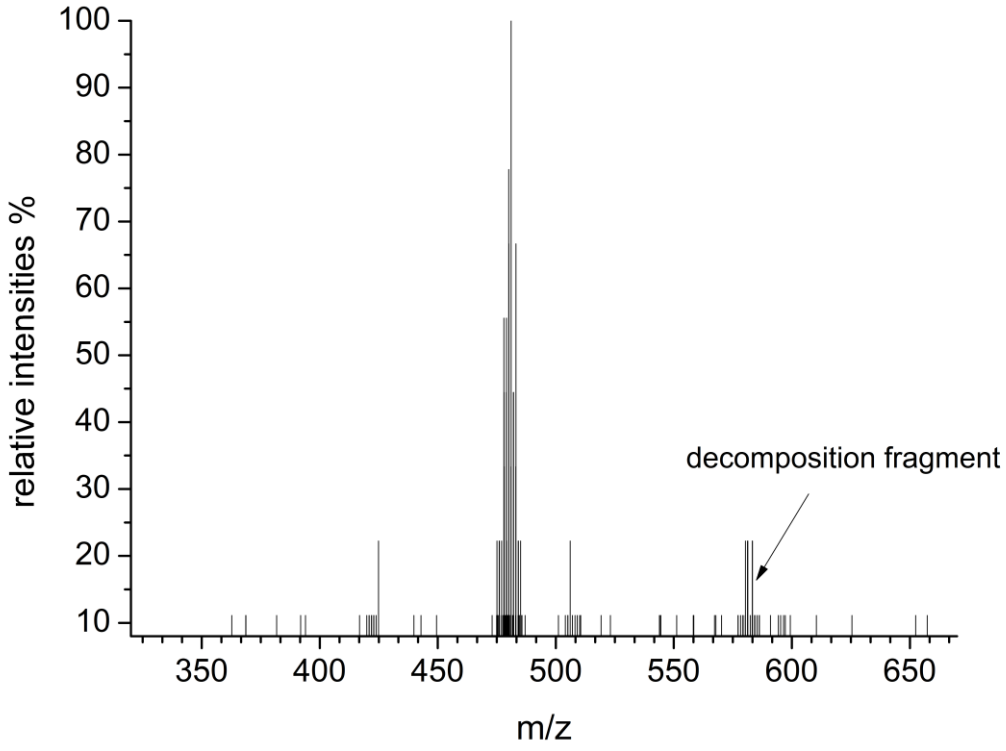

Figure S14 LIFDI-MS of [Ru(H_2)H_2(Me-PNP)] **6** in toluene. RT 2.16 min of 5.20 min.

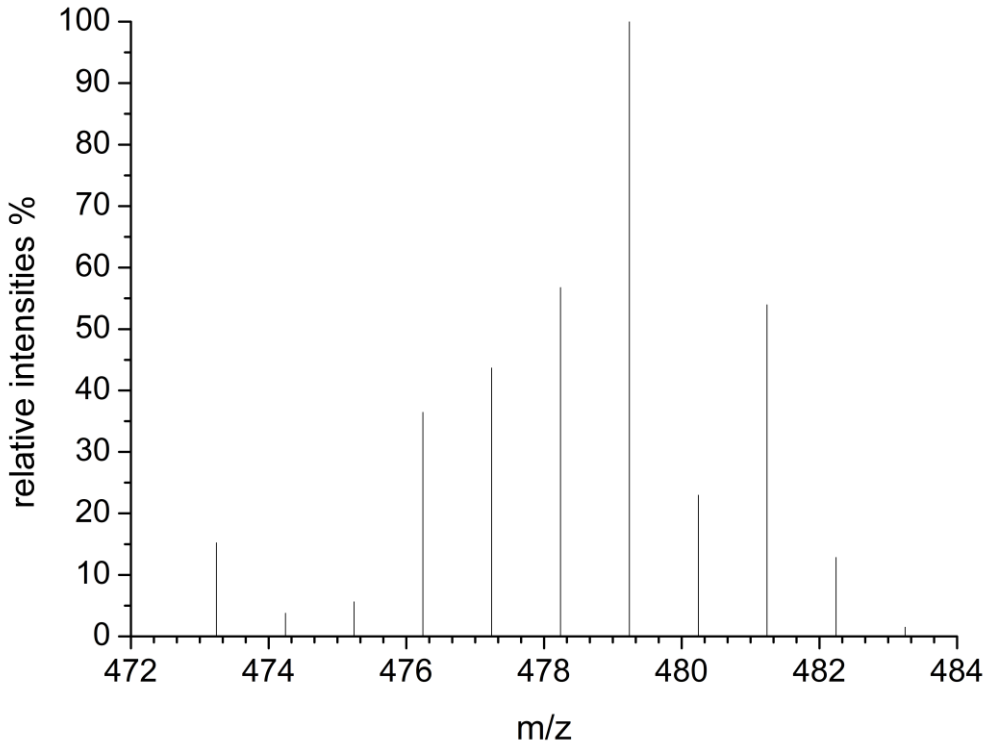

Figure S15 Simulated isotope pattern of [RuH_2(Me-PNP)] 479.

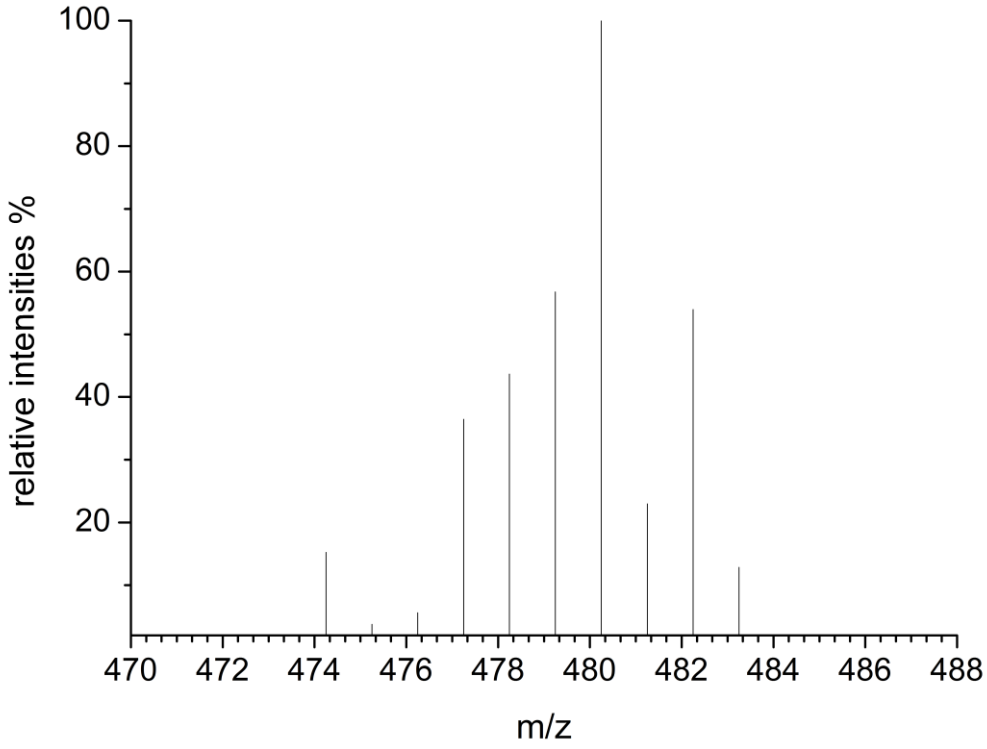

Figure S16 Simulated isotope pattern of [Ru(H_2)H(Me-PNP)] 480.

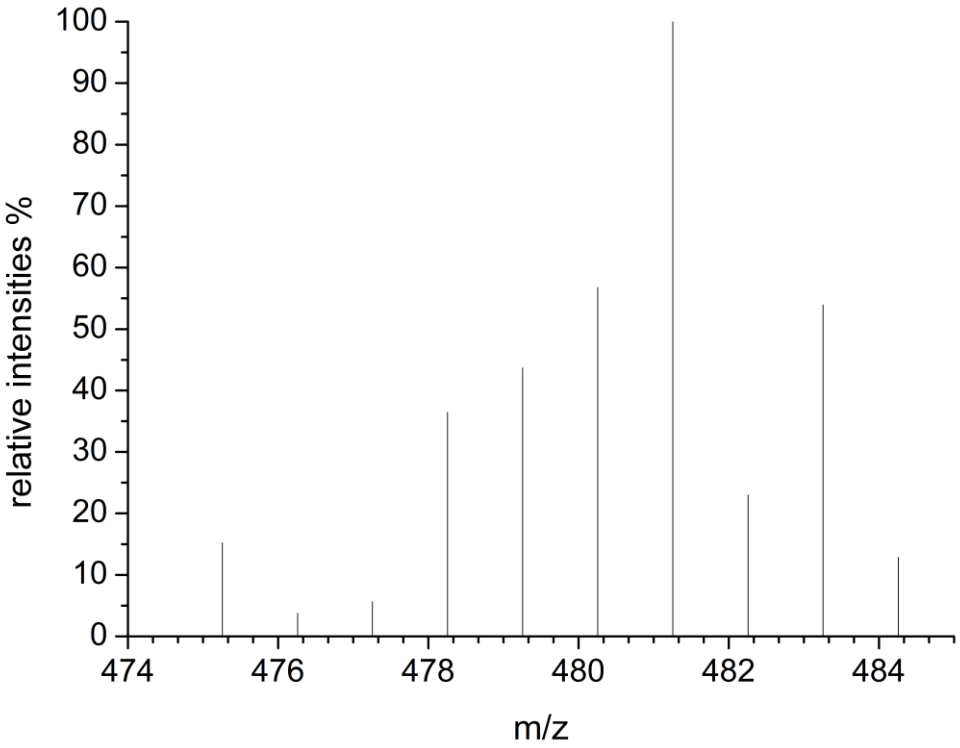

Figure S17 Simulated isotope pattern of [Ru(H_2)H_2(Me-PNP)] 481.

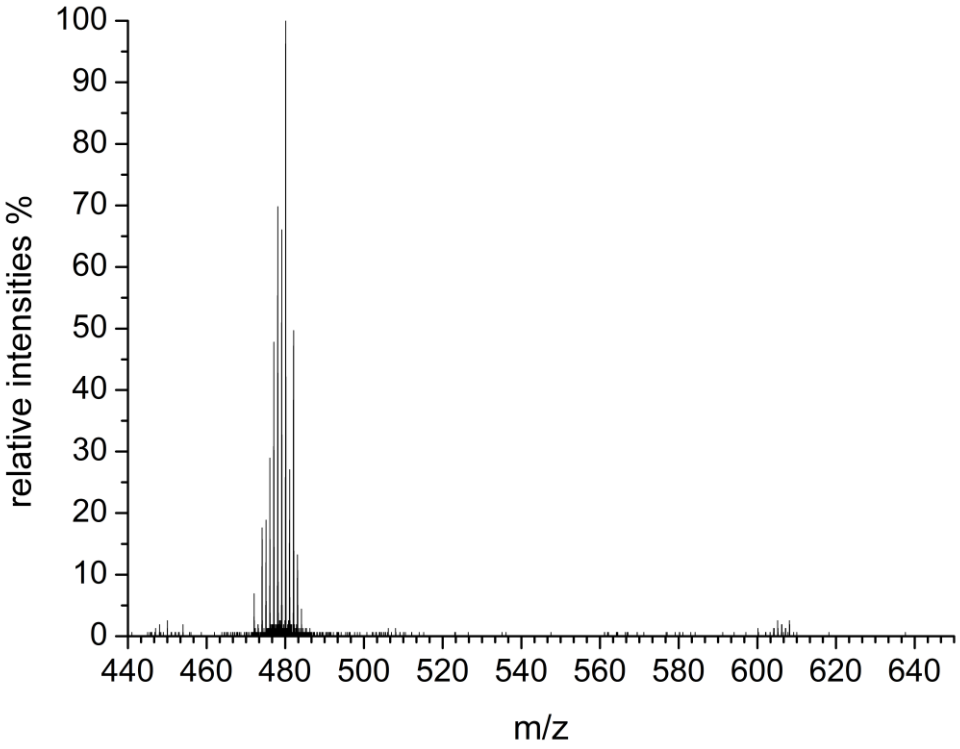

Figure S18 LIFDI-MS of [RuH_2(HBPin)(Me-PNP)] **10** in toluene. RT 2.04 min of 4.48 min

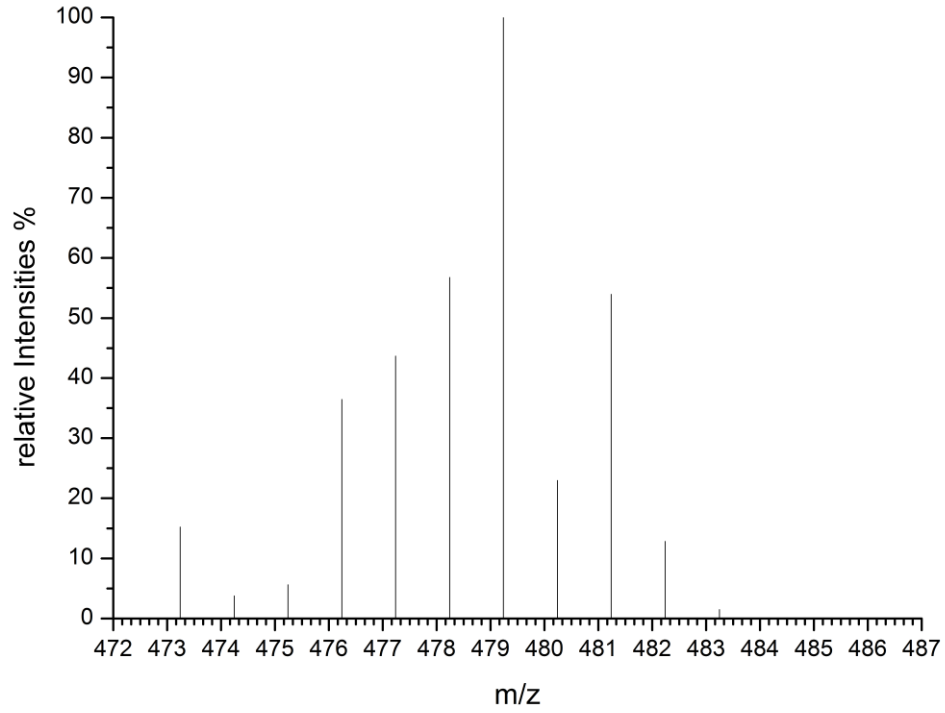

Figure S19 Simulated isotope pattern of fragment [RuH_2(Me-PNP)] 473 – 482.

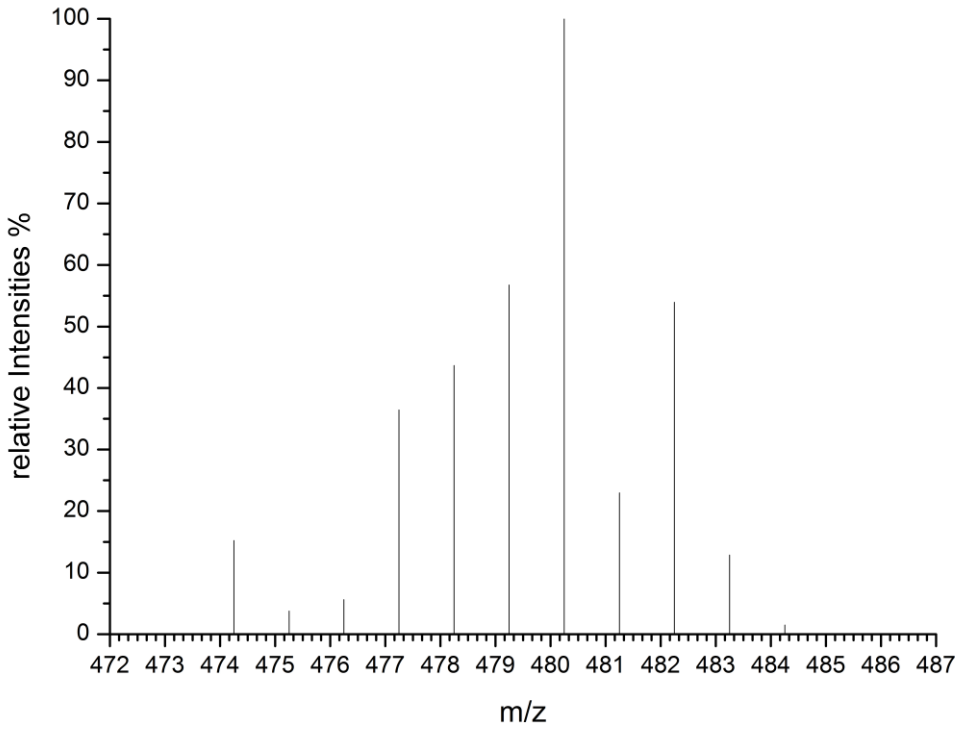

Figure S20 Simulated isotope pattern of fragment [RuH_3(Me-PNP)] 474 - 483.

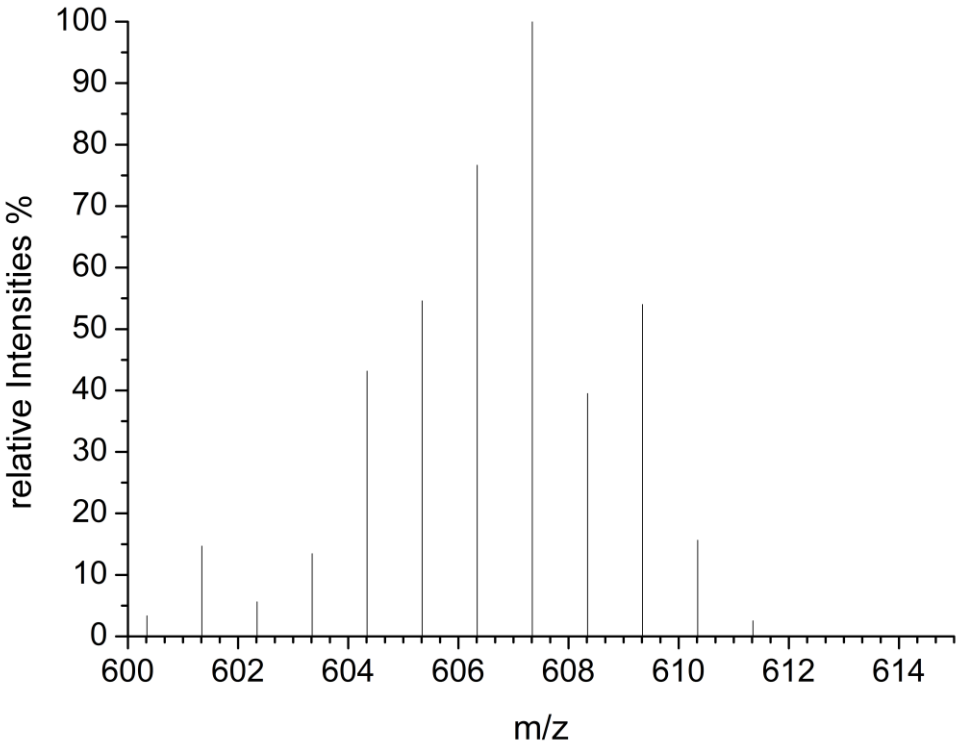

Figure S21 Simulated isotope pattern of RuH_2(HBPin)(Me-PNP)] 607.

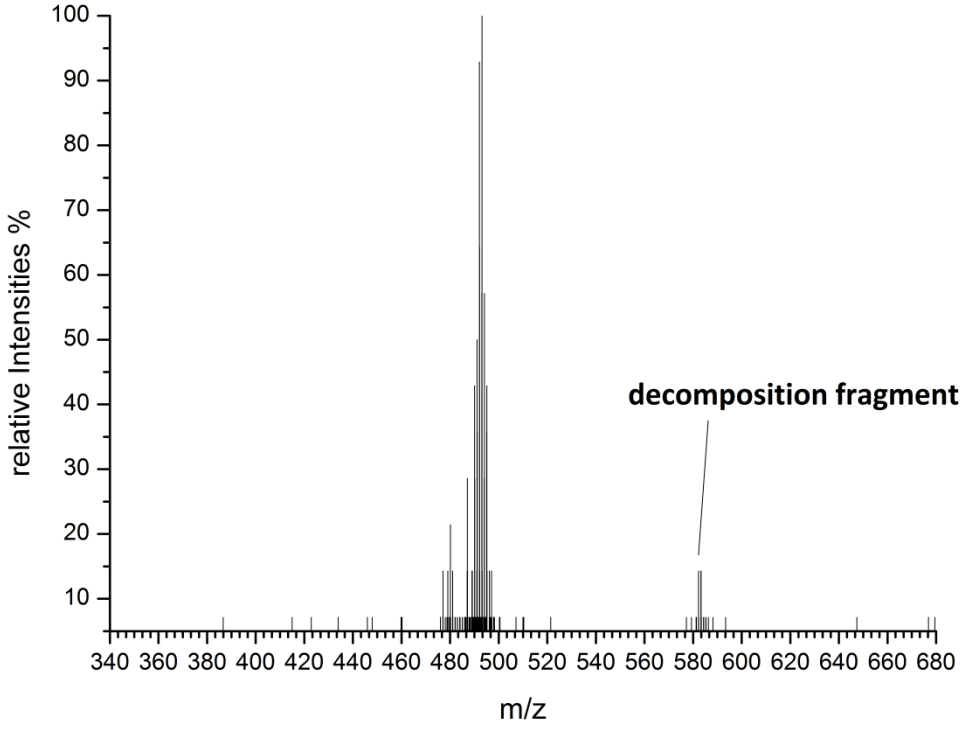

Figure S22 LIFDI-MS of [$RuH_2(BH_3)$(Me-PNP)] **11** in toluene. RT 1.51 min of 5.20 min.

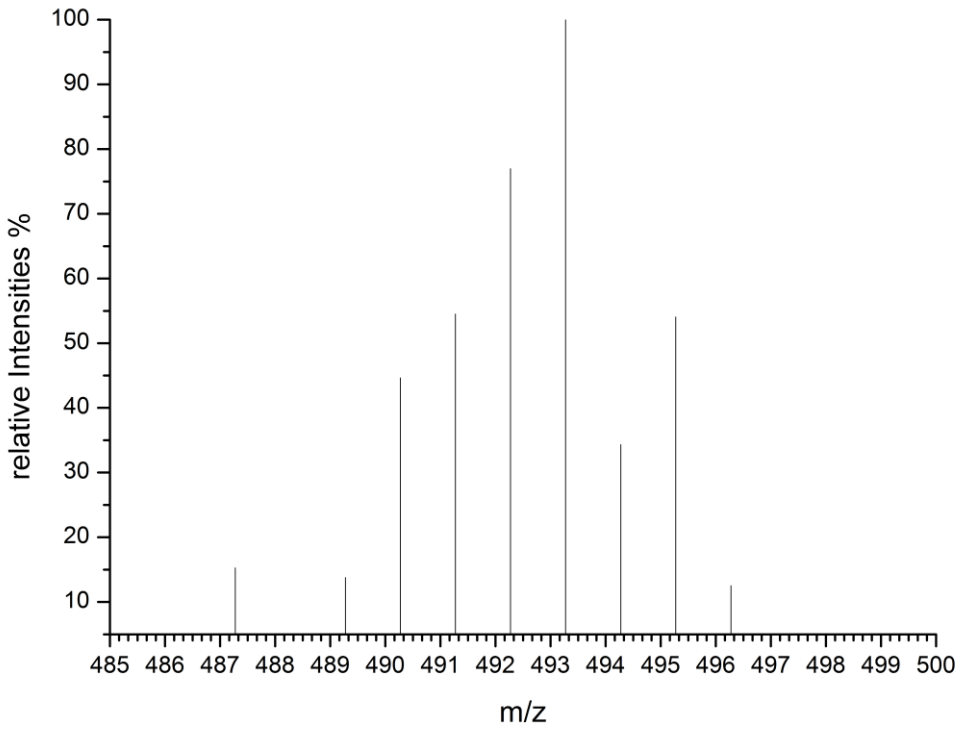

Figure S23 Simulated isotope pattern of [$RuH_2(BH_3)$(Me-PNP)] 493.

Crystallographic Data

Table 1. Crystallographic data of complex **11**

Compound	**11**
CCDC No.	952413
Formula	C21 H52 B N P2 Ru
M	492.46
Crystal System	Monoclinic
Space Group	C 2/c
T[K]	293
a[Å]	35.012(10)
b[Å]	8.148(5)
c[Å]	23.290(5)
α[deg]	90
β[deg]	125.001(14)
γ[deg]	90
V[Å^3]	5442(4)
Z	8
Density [gcm^{-3}]	1.202
μ(mm^{-1})	0.700
Θ range[deg]	0.983≤ θ ≤27.35
No. of reflections measured	31439
No. of independent reflections	6060
Reflns collected	2749
R_{int}	0.1306
Completeness	0.983
Final R_1 values [all data]	0.1476
wR_2[all data]	0.1201
GoF	0.902

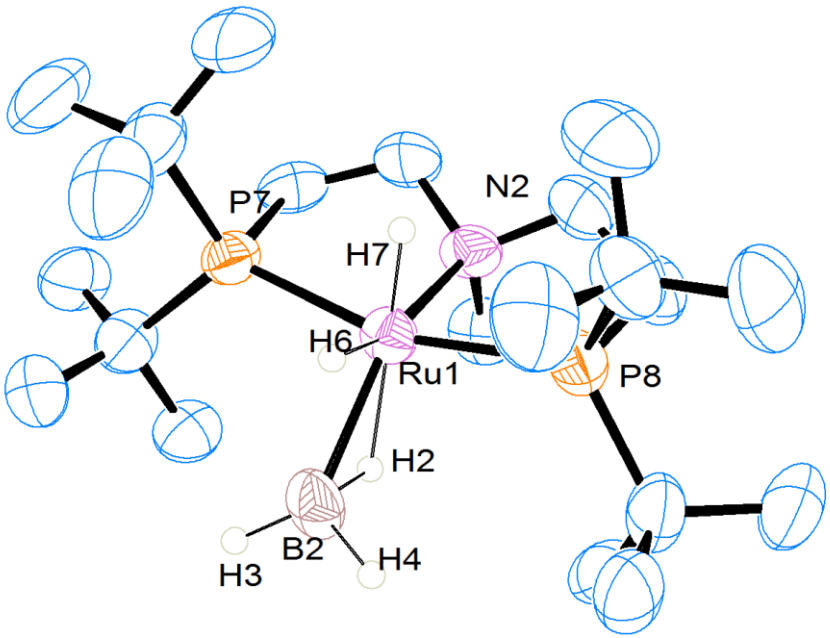

Figure S24 ORTEP diagram of the single crystal structure of complex **11**. Ellipsoids are illustrated at 50% possibility. All hydrogen atoms are faded out except for H7, H6, H4, H3 and H2 for clarity.

Table 2 Selected bond distances [Å] and angles [deg].

Ru1-P7	2.33(3)	P7-Ru1-P8	163.06
Ru1-P8	2.32(7)	Ru1-H2-B2	92.76
Ru1-N2	2.18(9)	H7-Ru1-H2	170.78
Ru1-H7	1.36(6)	H7-Ru1-P7	63.28
Ru1-H6	1.48(8)	H7-Ru1-P8	65.96
Ru1-H2	1.69(2)	N2-Ru1-B2	143.08
Ru1-B1	2.19(2)	H3-B1-H4	108.16
B1-H2	1.31(6)		
B1-H6	1.84(2)		
B1-H3	1.04(6)		
B1-H4	1.15(7)		

Calculated with SXGRAPH SHELX Graphical Editor.