Electronic Supplementary Material (ESI) for Dalton Transactions. This journal is © The Royal Society of Chemistry 2015

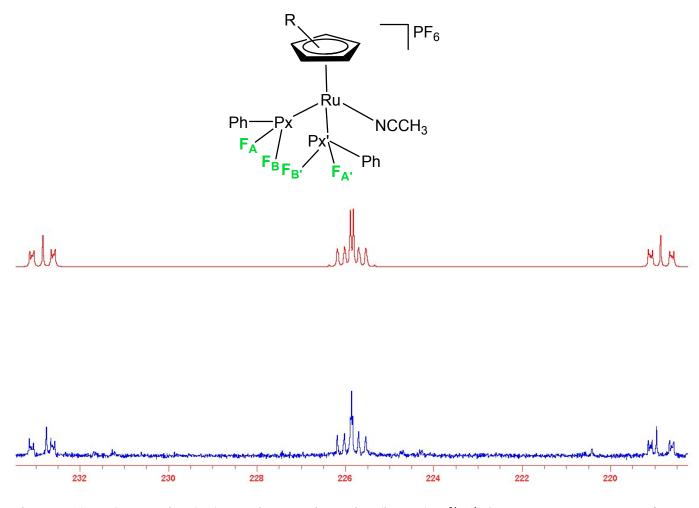


Figure 1S. Computed (top) and experimental (bottom) ${}^{31}P{}^{1}H$ NMR spectrum of $[(C_5Me_5)Ru(CH_3CN)(PhPF_2)_2]PF_6$ (acetone-d₆, 161.89 MHz, 294 K)

Table 1S. Calculated values for coupling constants *J* for $[(C_5Me_5)Ru(CH_3CN)(PhPF_2)_2]PF_6$. Labels are taken from Figure 1S.

Nucleus	δ(ppm)	P _{X'}	F _A	F _B	F _{A'}	F _{B'}
P _x	225.85	78.38	1143.75	-1117.90	-9.36	-4.36
P _{X'}	225.85		-5.36	-9.36	1143.75	-1117.90
F _A				48.70		
F _B						
F _Β ,						42.0