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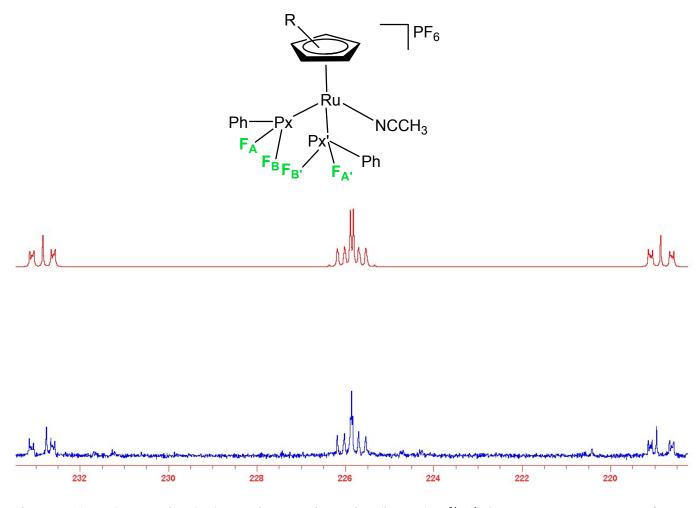


Figure 1S. Computed (top) and experimental (bottom)  ${}^{31}P{}^{1}H$  NMR spectrum of  $[(C_5Me_5)Ru(CH_3CN)(PhPF_2)_2]PF_6$  (acetone-d<sub>6</sub>, 161.89 MHz, 294 K)

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 <sub>X'</sub>	F <sub>A</sub>	F <sub>B</sub>	F <sub>A'</sub>	F <sub>B'</sub>
P <sub>x</sub>	225.85	78.38	1143.75	-1117.90	-9.36	-4.36
P <sub>X'</sub>	225.85		-5.36	-9.36	1143.75	-1117.90
F <sub>A</sub>				48.70		
F <sub>B</sub>						
F <sub>Β</sub> ,						42.0