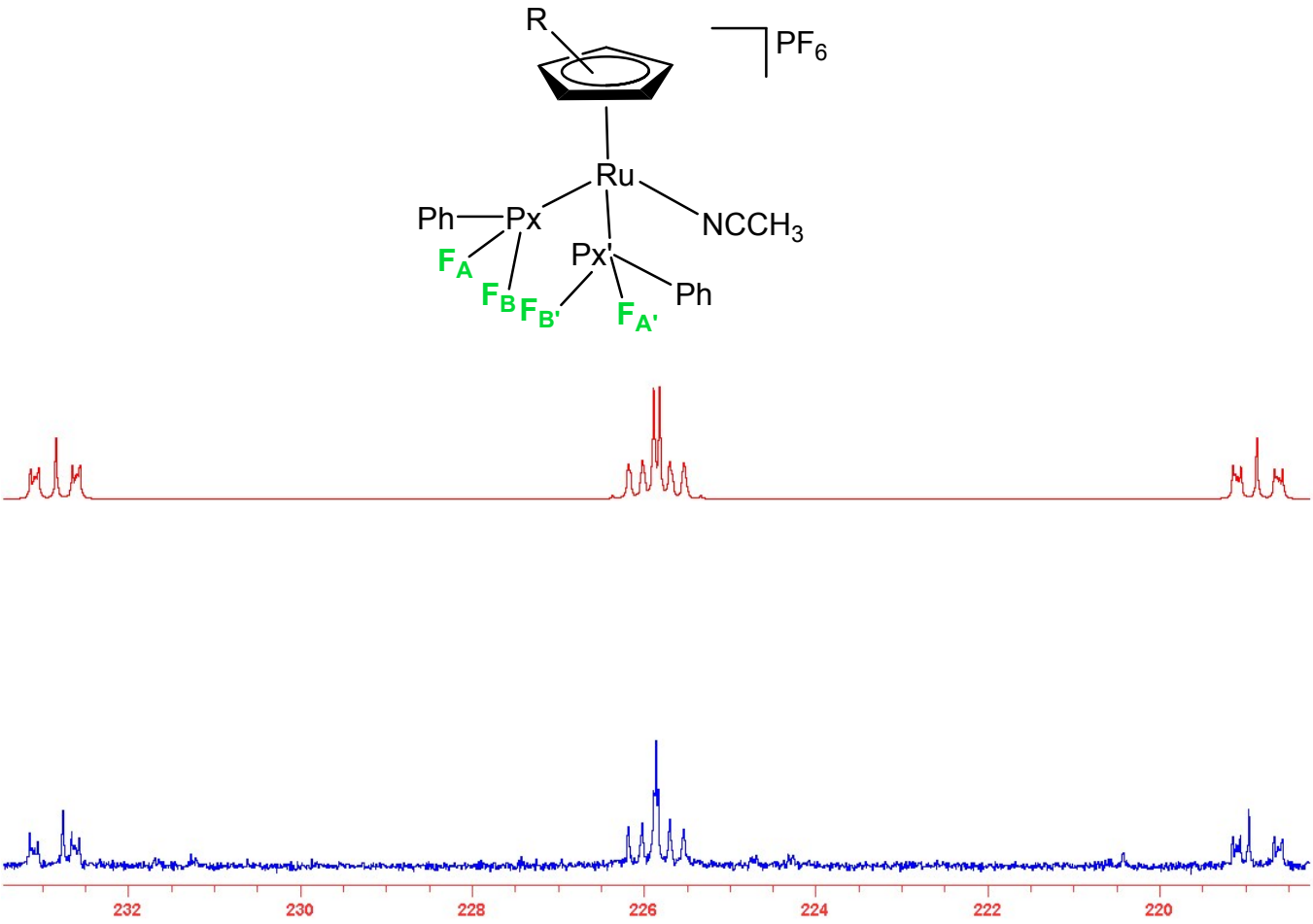

Figure 1S. Computed (top) and experimental (bottom) $^{31}P\{^{1}H\}$ NMR spectrum of $[(C_5Me_5)Ru(CH_3CN)(PhPF_2)_2]PF_6$ (acetone-d_6, 161.89 MHz, 294 K)

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	---			---	---	---
$F_{B'}$	---				---	42.0