Supporting Information:

Synthesis and Characterization of Ruthenium Bis(β-diketonato) Pyridine-Imidazole Complexes for Hydrogen Atom Transfer

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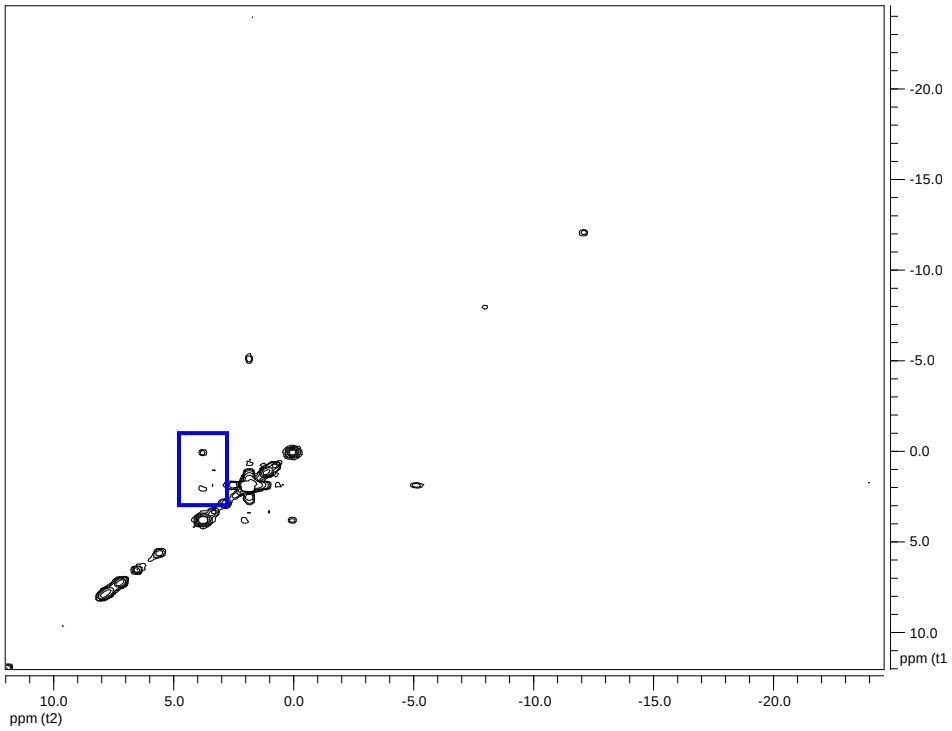

Figure S1. ^{1}H 2D COSY NMR spectrum of [Ru^{III}(acac)$_2$(py-imH)]OTf (**2**) in CD_3CN. The two cross peaks (δ 3.91 couples to δ 0.07 and 2.14) are highlighted in the rectangular box.

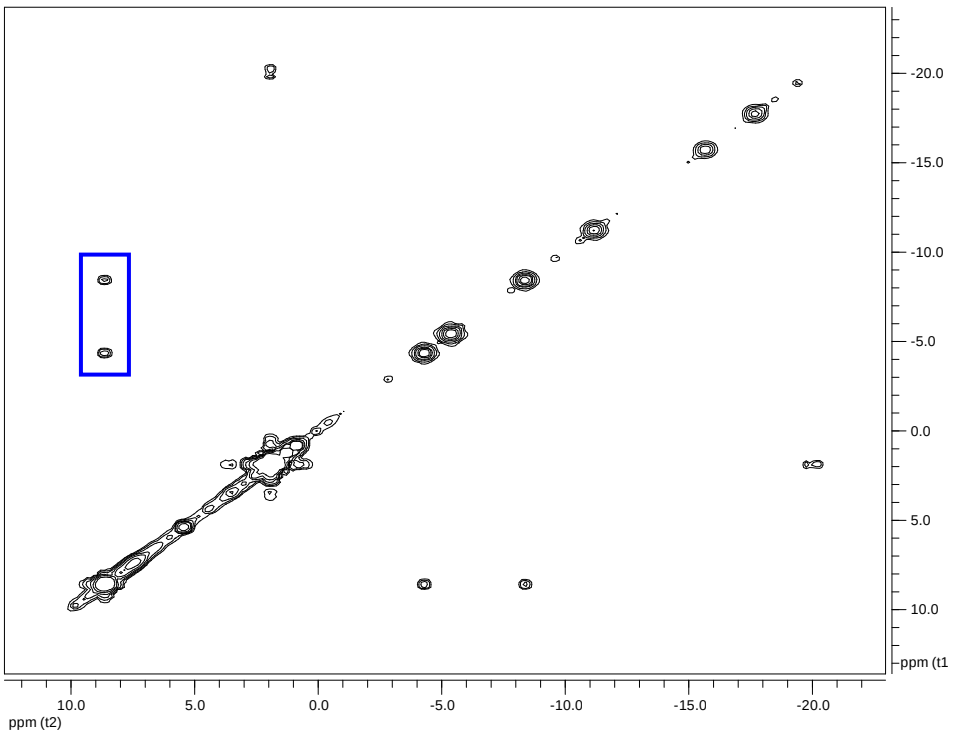

Figure S2. ^{1}H 2D COSY NMR spectrum of $Ru^{III}(acac)_2$(py-im) (**3**) in CD_3CN. The two cross peaks (δ 8.75 couples to δ –8.56 and –4.46) are highlighted in the rectangular box.

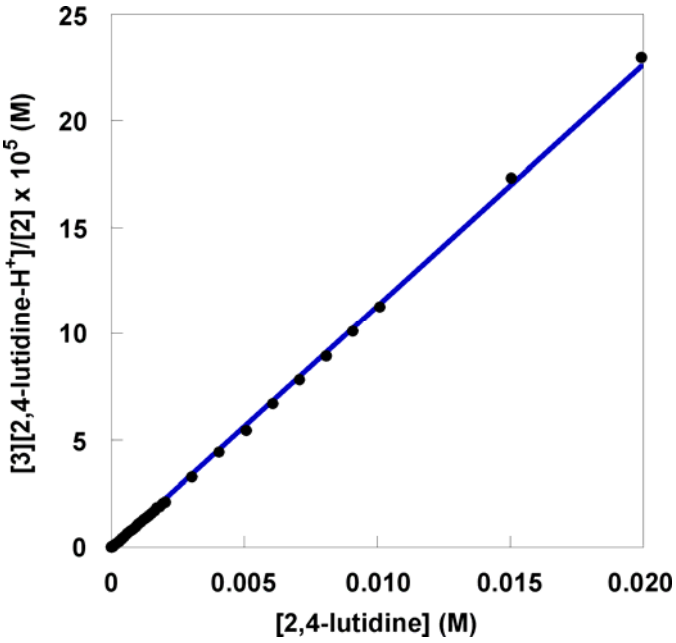

Figure S3. Plot of [**3**][2,4-lutidine-H^+]/[**2**] vs. [2,4-lutidine] for the equilibrium titration: [$Ru^{III}(acac)_2$(py-imH)]OTf (**2**) + 2,4-lutidine ⇄ $Ru^{III}(acac)_2$(py-im) (**3**) + (2,4-lutidine-H)OTf in MeCN. The slope of the linear plot (R^2 = 0.999) is the equilibrium constant K_{eq} = 0.011 ± 0.001.

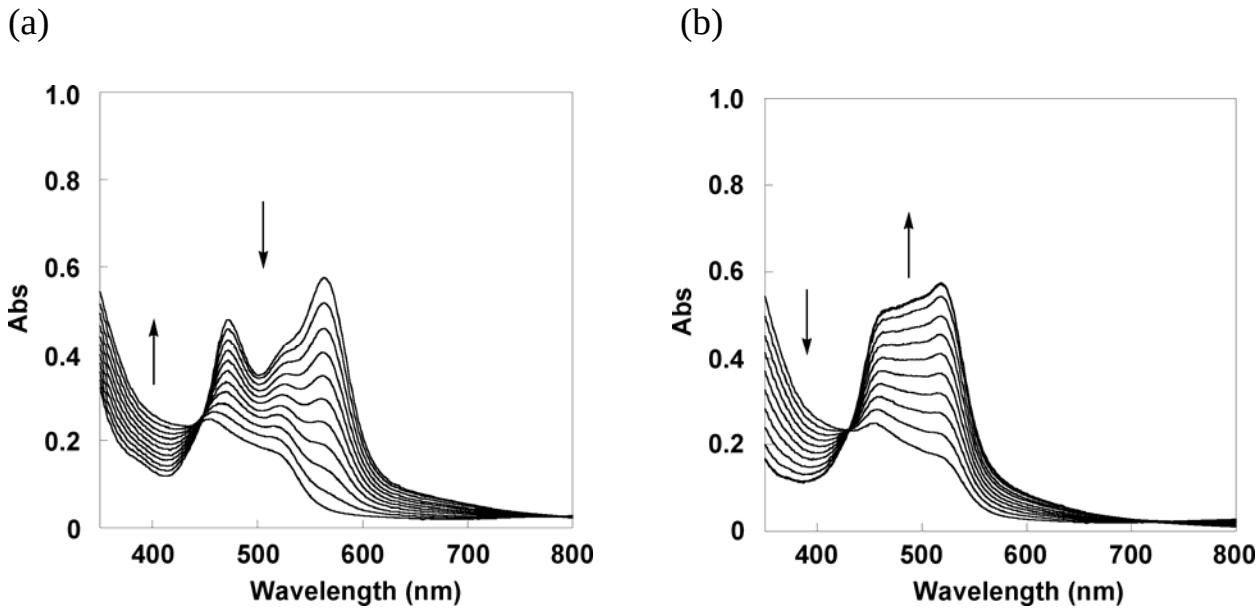

Figure S4. UV-vis titration plots of (a) [DBU-H][Ru^{II}(hfac)$_2$(py-im)] (**5**) (0.053 mM) + 1 equiv of [N(tol)$_3$]PF_6 in MeCN to generate Ru^{III}(hfac)$_2$(py-im) (**6**) and (b) further titration of **6** + 1 equiv of TEMPO–H to produce Ru^{II}(hfac)$_2$(py-imH) (**4**).

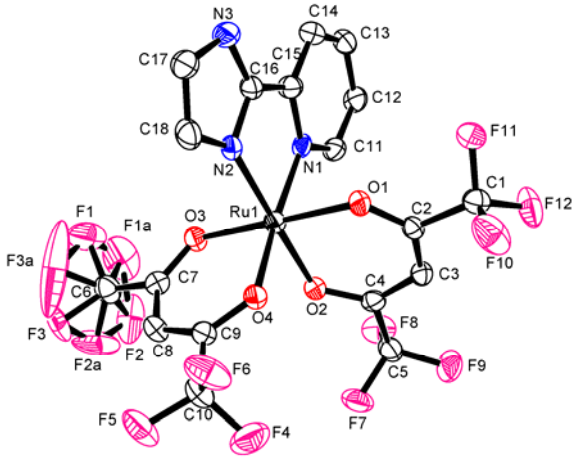

Figure S5. ORTEP drawing of [Ru^{II}(hfac)$_2$(py-im)]$^-$ (**5**) showing both the major 80% (F1, F2, and F3) and minor 20% (F1A, F2A, and F3A) occupancies of the disordered CF_3 group.