

Synthesis and characterization of ruthenium polypyridyl complexes with hydroxypyridine derivatives: Effect of protonation and ethylation at the pyridyl nitrogen

Juyeong Kim, Hemant P. Yennawar, and Benjamin J. Lear*

Department of Chemistry, The Pennsylvania State University, University Park, Pennsylvania 16802, United States

Contents

Title	Page
Fig. S1 UV-visible spectrum of 1	S2
Fig. S2 UV-visible spectra of 1, 2, and 3	S2
Fig. S3 Emission spectra of 1	S3
Fig. S4 Full NMR spectrum of 1	S4
Fig. S5 Aromatic region of NMR spectrum of 1	S4
Fig. S6 Selected NMR spectra of 1 with addition of NaOH	S5
Fig. S7 Cyclic voltammograms of 1, 2, and 3	S6
Fig. S8 Reductive differential pulse voltammograms of 1, 2, and 3	S7
Fig. S9 Cyclic voltammogram of 2,3'-dihydroxypyridine	S7
Fig. S10 Full spectral overlays from the spectroelectrochemistry of 3^0 and 3^{1-}	S8

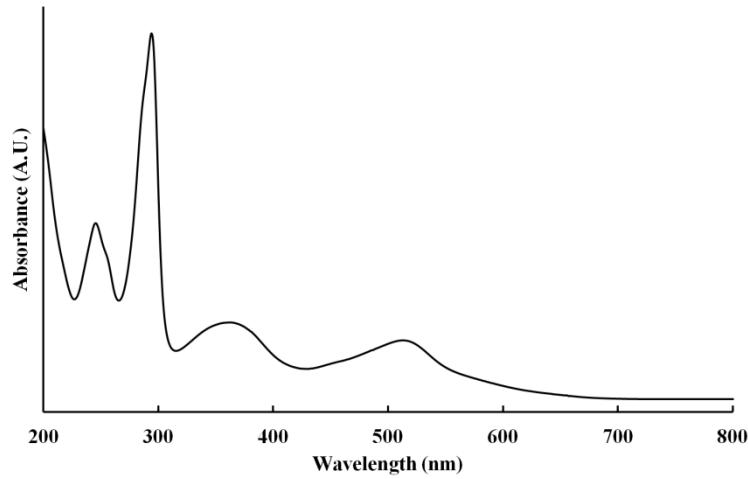


Fig. S1 UV-visible spectrum of **1** in distilled water at 298 K.

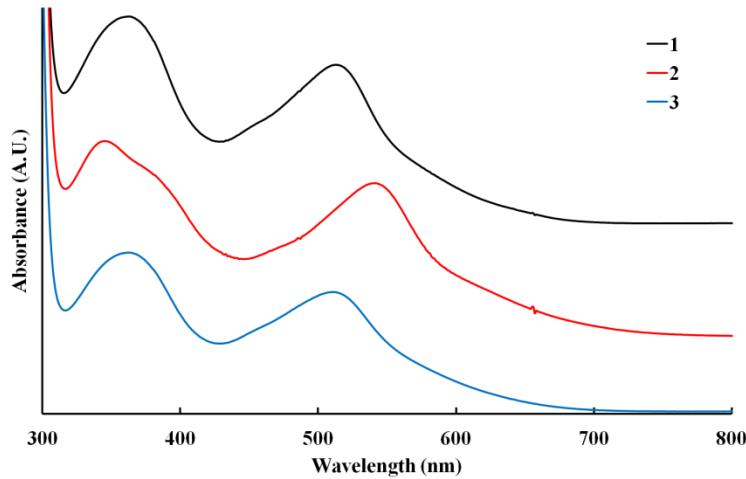


Fig. S2 UV-visible spectra of **1** (black line), **2** (red line), and **3** (blue line) in distilled water at 298 K.

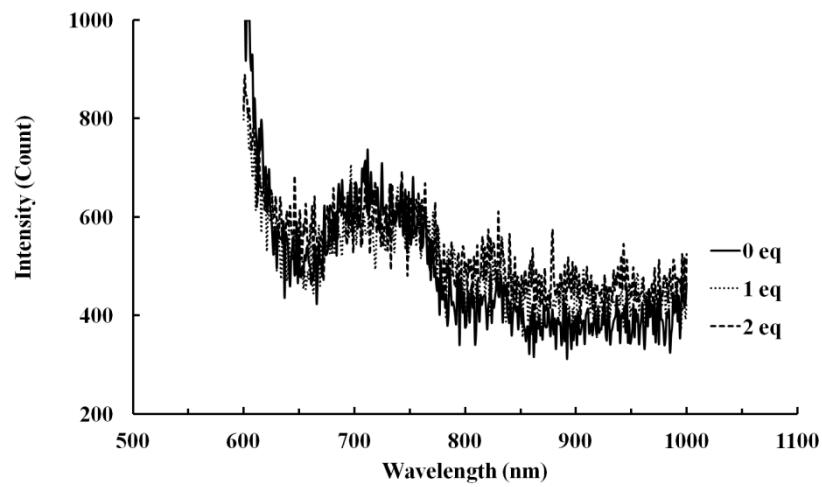


Fig. S3 Emission spectra of **1** with 0, 1, and 2 equivalents of 0.02 M NaOH in DMSO at 298 K.

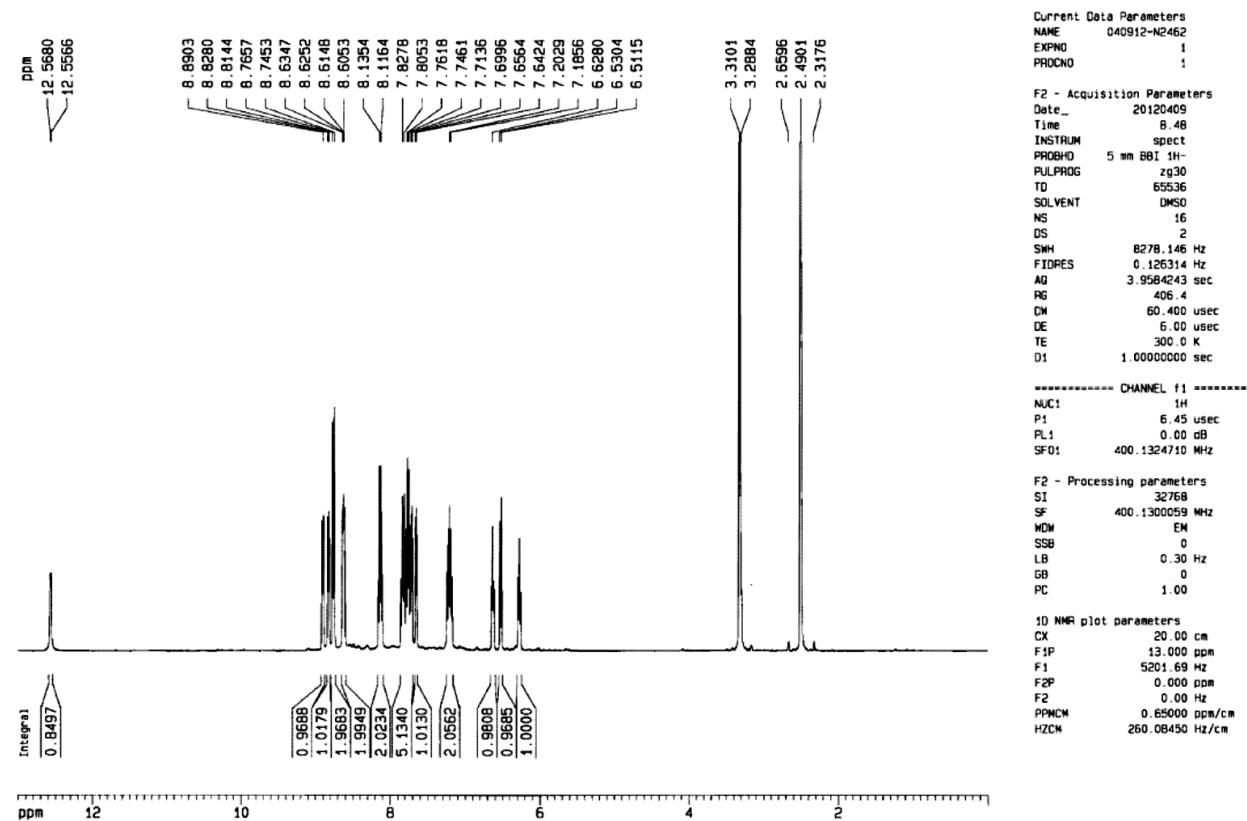


Fig. S4 Full NMR spectrum of **1** in C₂D₆OS.

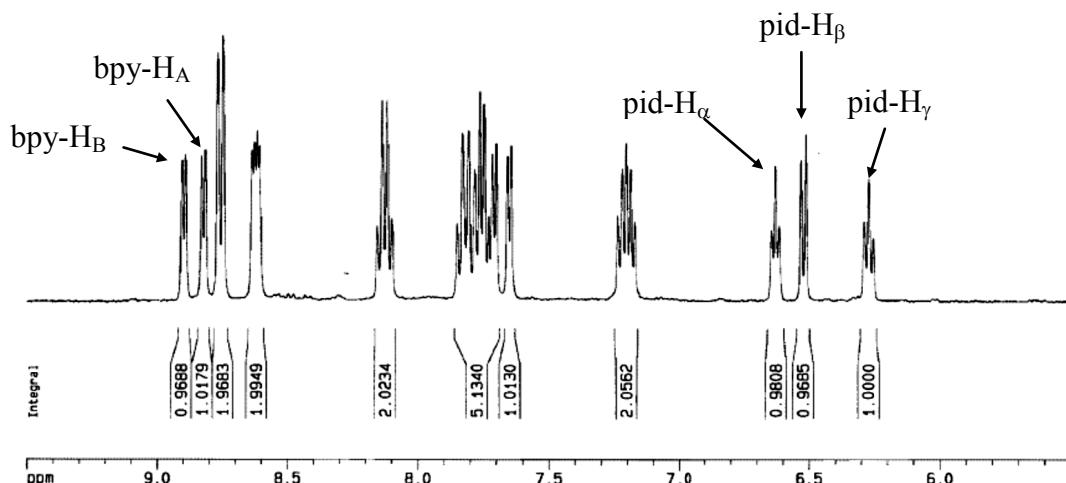


Fig. S5 Aromatic region of NMR spectrum of **1** in C₂D₆OS with assignments of related proton signals.

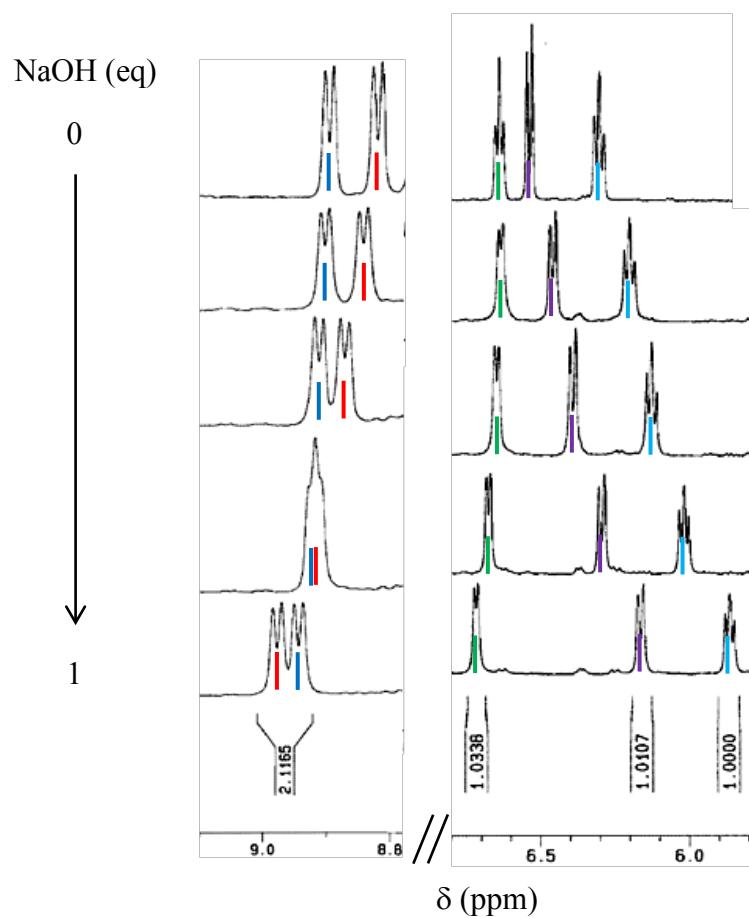


Fig. S6 Selected NMR spectra of **1** in $\text{C}_2\text{D}_6\text{OS}$ with addition of NaOH (0, 0.25, 0.5, 0.75, and 1 eq). Each color represents H_A (red line), H_B (blue line), H_α (green line), H_β (light blue line), and H_γ (purple line).

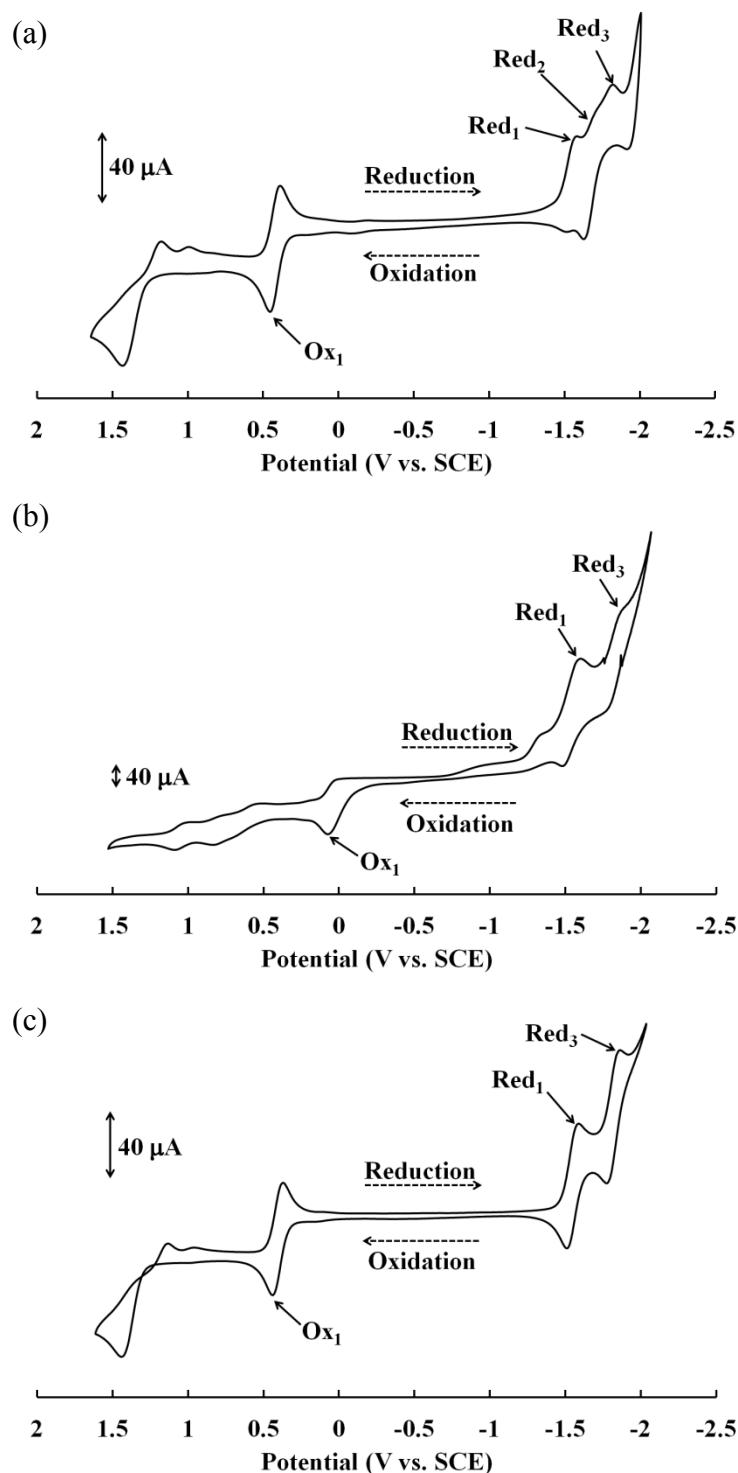


Fig. S7 Cyclic voltammograms of (a) **1**, (b) **2**, and (c) **3** in acetonitrile/0.1 M NBu₄PF₆ at 298 K.
Scan rate: 100 mVs⁻¹. Each cycle started at 0 V towards the positive potential.

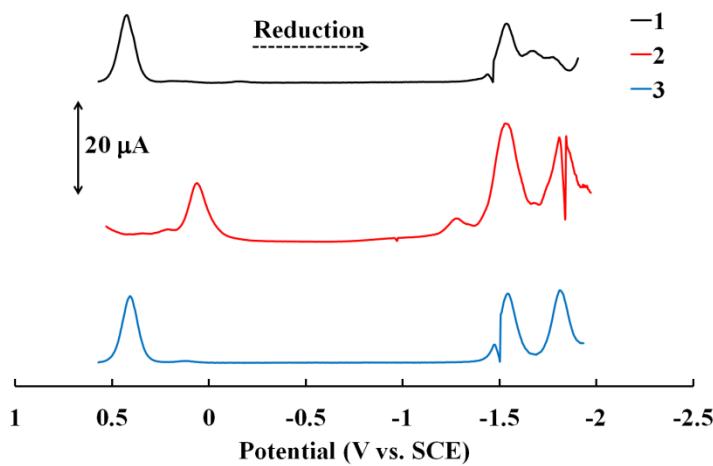


Fig. S8 Reductive differential pulse voltammograms of **1** (black line), **2** (red line), and **3** (blue line) in acetonitrile/0.1 M NBu₄PF₆ at 298 K. Scan rate: 4 mVs⁻¹.

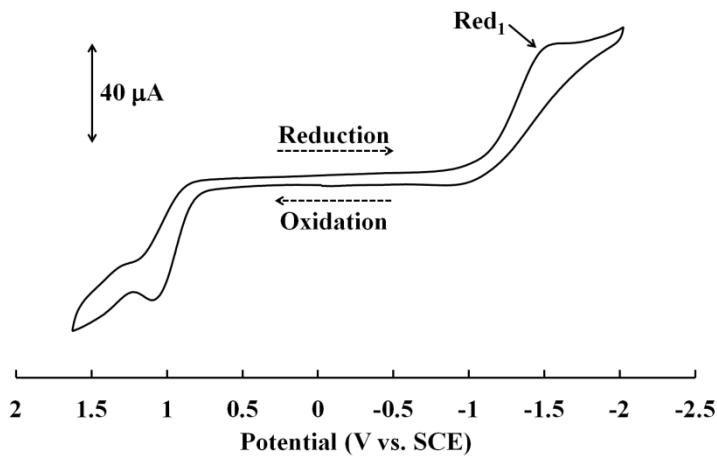


Fig. S9 Cyclic voltammogram of 2,3'-dihydroxypyridine in acetonitrile/0.1 M NBu₄PF₆ at 298 K. Scan rate: 100 mVs⁻¹. The scan started at 0 V towards the positive potential.

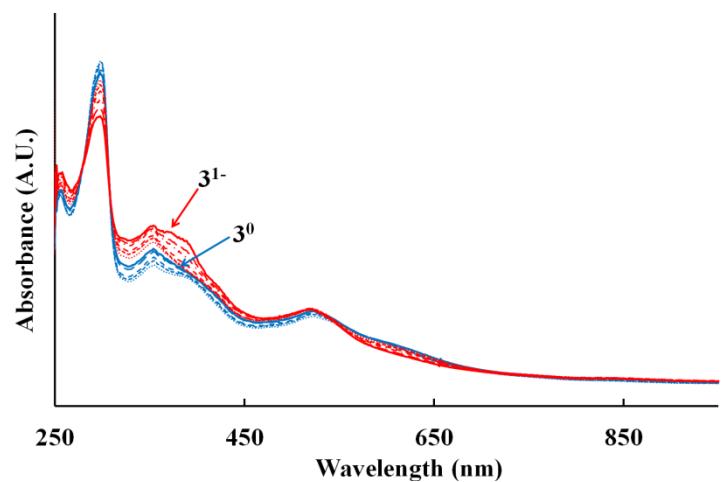


Fig. S10 Full spectral overlays from the spectroelectrochemistry of 3^0 (blue line) and 3^{1-} (red line) in DMSO/0.1M NBu_4PF_6 at 298 K.