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Supporting information for article:

Structural and electrochemical comparison of trinuclear ruthenium oxo clusters $[\text{Ru}_3(\text{OAc})_6\text{O}(\text{L})_3]^+$ and $[\text{Ru}_3(\text{OAc})_6\text{O}(\text{L})_2(\text{CO})]$ (L = imidazole, benzimidazole, and 4-phenylpyridine)

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S1. Cyclic voltammograms

Figure S1 Cyclic voltammograms of **[2]PF₆** in (a) acetonitrile and (b, c) 9:1 CH₂Cl₂:MeOH with 0.1 M TBAPF₆, glassy carbon working electrode, Ag/AgCl reference electrode, and Pt wire counter electrode. (a) A full range scan (200 mV/s) shows the irreversible behaviour at -1.35 V; (b) Narrow range scans (50, 100, and 200 mV/s) show two reversible redox couples; (c) Multiple scans at 200 mV/s in the range of 0.5 to -2.0V show the appearance of new species at ~ -0.26V.

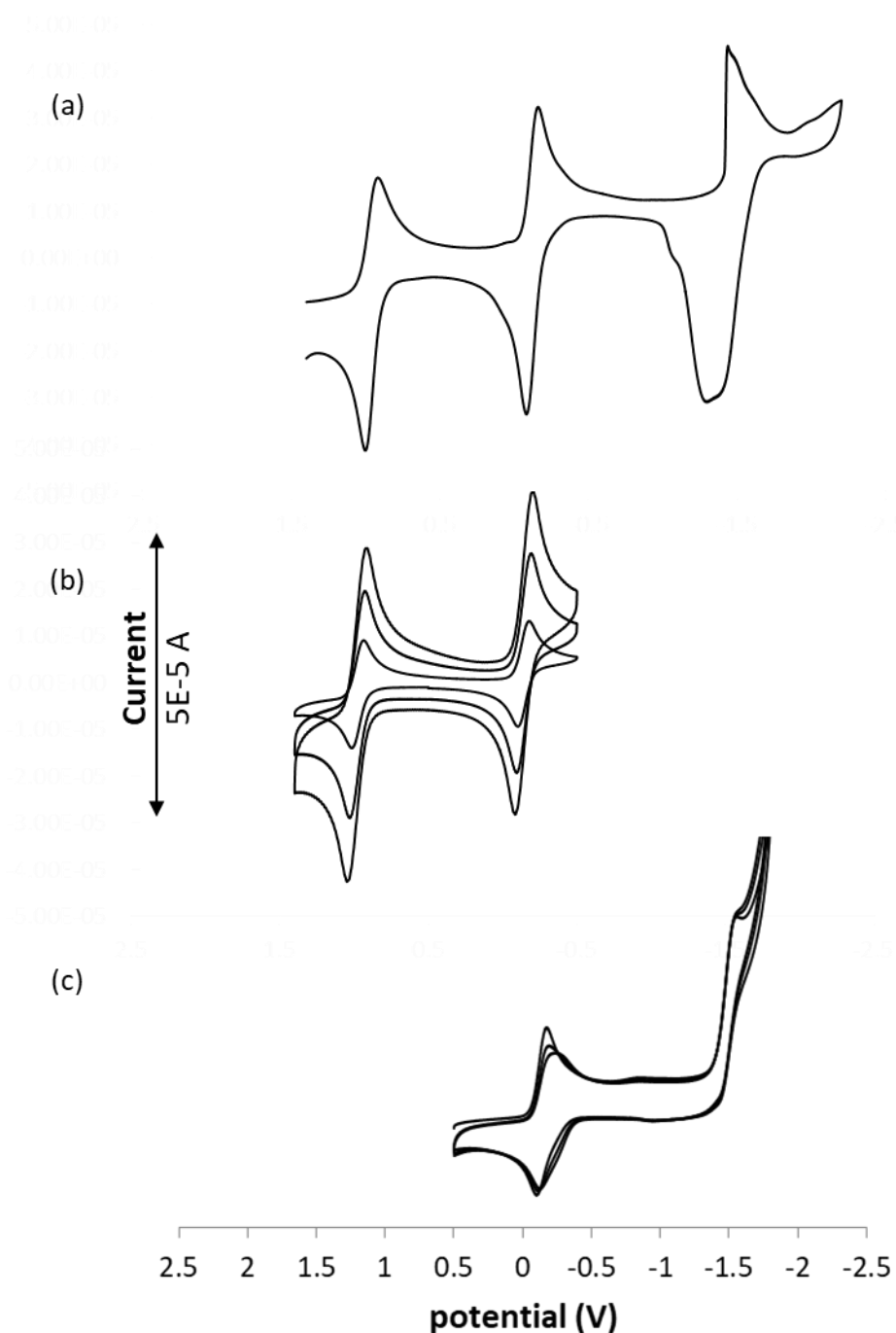


Figure S2 Cyclic voltammogram of **[3]PF₆** in acetonitrile with 0.1 M TBAPF₆, glassy carbon working electrode, Ag/AgCl reference electrode, and Pt wire counter electrode, scan rate 100 mV/s. The couple with $E_{1/2} = -1.65$ V is ligand-based.

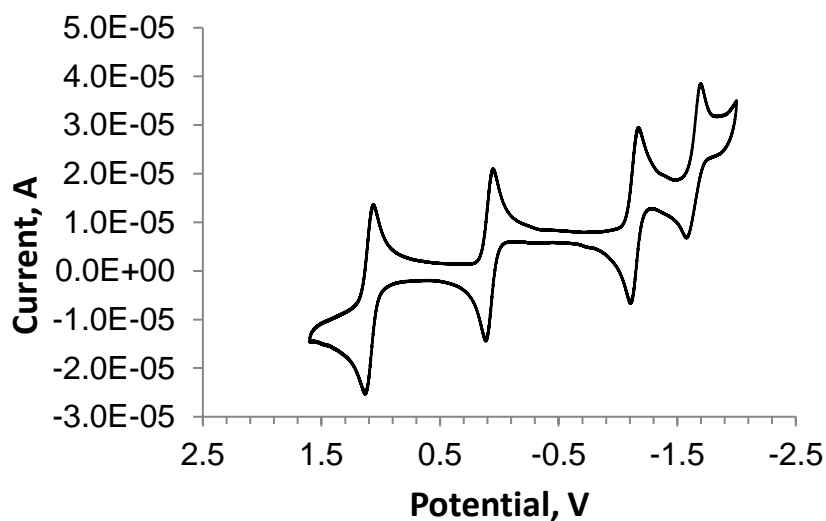


Figure S3 Cyclic voltammogram of 4-phenylpyridine in acetonitrile with 0.1 M TBAPF₆, glassy carbon working electrode, Ag/AgCl reference electrode, and Pt wire counter electrode, scan rate 500 mV/s

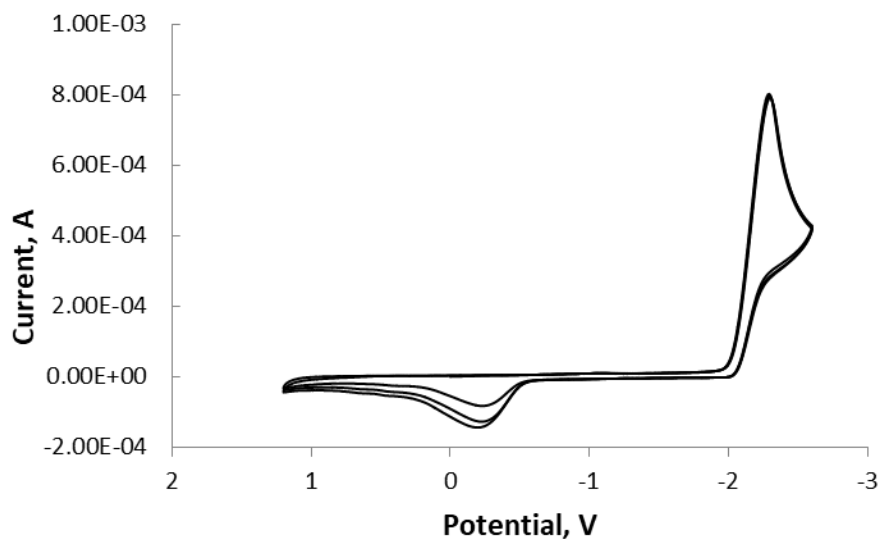


Figure S4 ESI mass spectra of reaction mixture taken at 30 min, 1, 3, and 12 h show imidazole coordination to $[\text{Ru}_3\text{O}(\text{OAc})_6(\text{H}_2\text{O})_3]^+$ to form occurs quickly (red asterisk), but does not reach completion during this time scale. Many peak envelopes are observed due to the various solvated forms of the cluster.

