

Supporting Information for:

**Electrochemical properties and C-H bond oxidation activity of [Ru(tpy)(pyalk)Cl]⁺
and [Ru(tpy)(pyalk)(OH)]⁺**

C. K. Nilles,^a H. Herath,^a H. Fanous,^a Angel Ugrinov^a and A. R. Parent^a

^a Department of Chemistry and Biochemistry, North Dakota State University, PO Box 6050, Fargo ND 58108-6050

Contents:

Supplemental Electrochemical Data	2-3
ESI-MS of [1]Cl	4-5
Light and Air dependence on C-H bond oxidation activity of 2	6

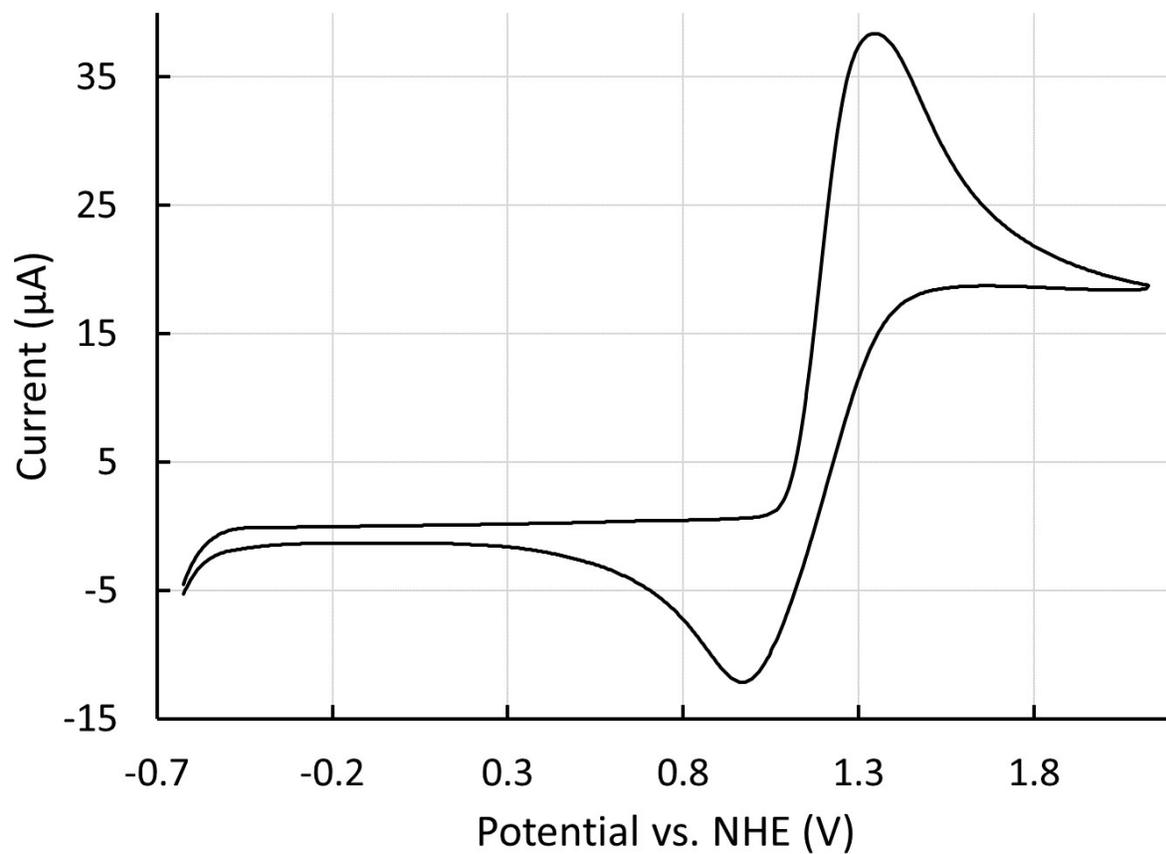


Figure S1. Cyclic voltammogram of 9.85 mM tetramethylammonium chloride at 50 mV/s in acetonitrile containing 100 mM tetra-N-butylammonium hexafluorophosphate as electrolyte.

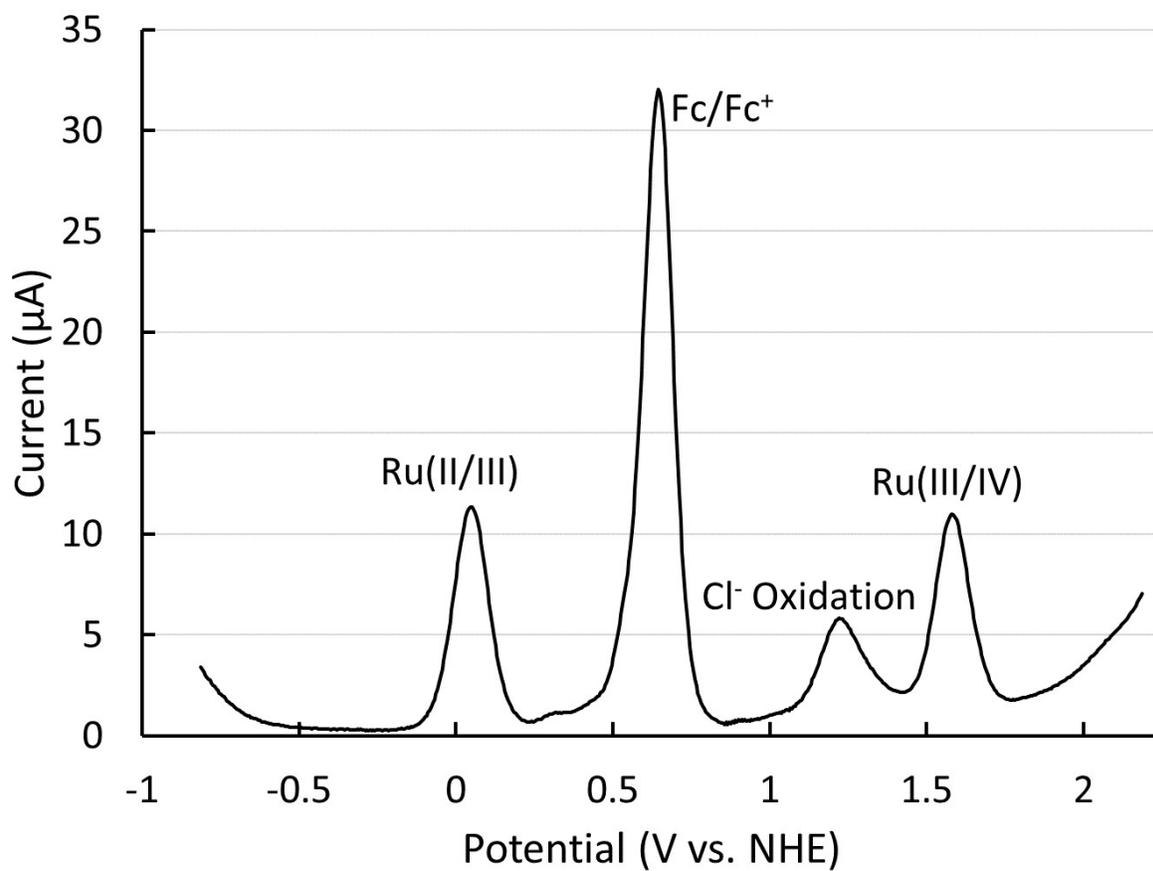


Figure S2. Differential pulse voltammogram of 2.5 mM [1]Cl in acetonitrile containing Fc as a reference and 100 mM tetra-N-butylammonium hexafluorophosphate as electrolyte.

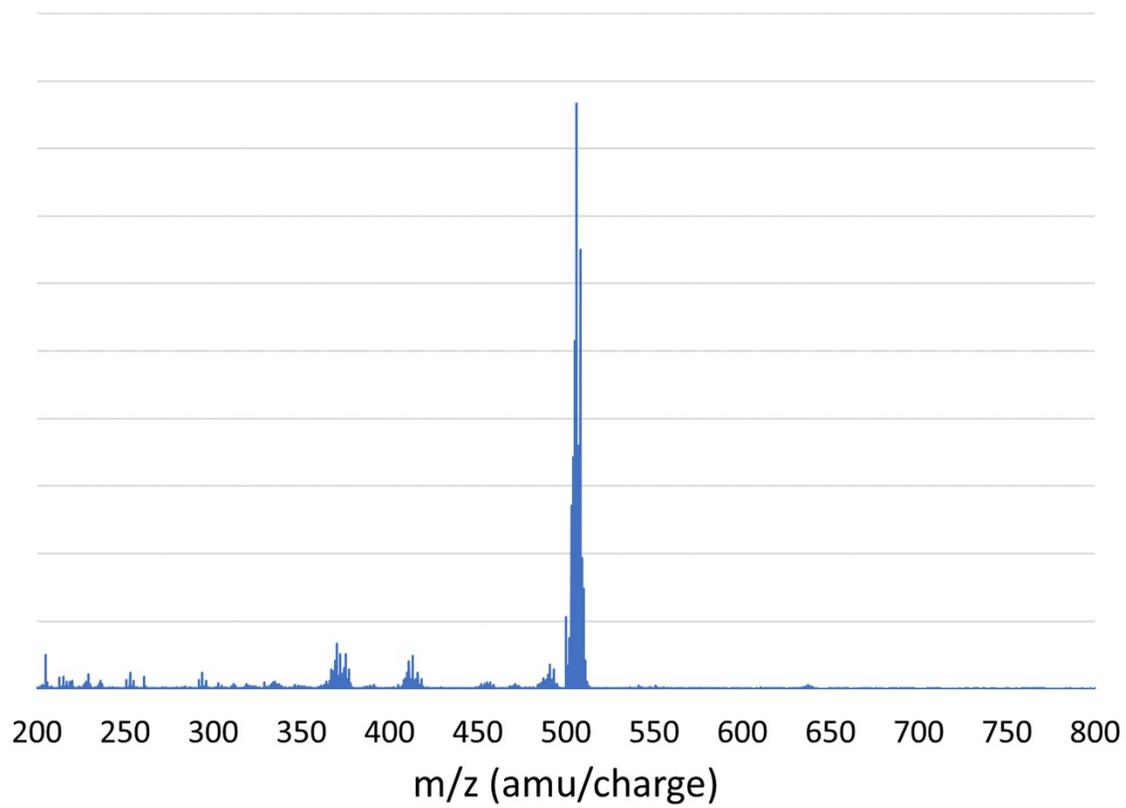


Figure S3. ESI-MS of [1]Cl in MeOH.

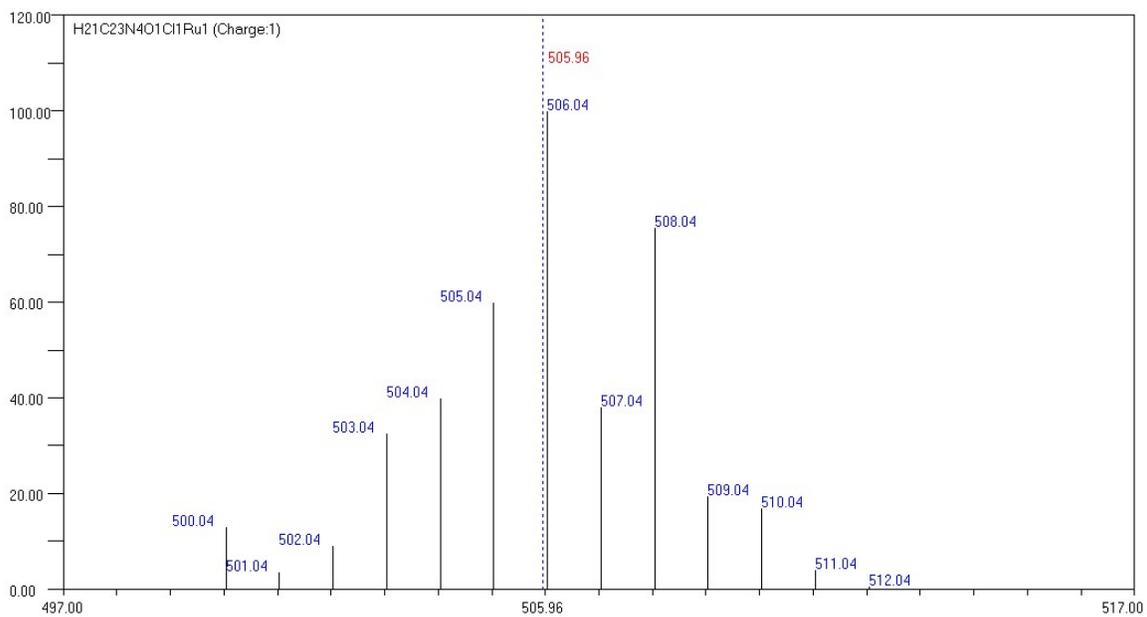
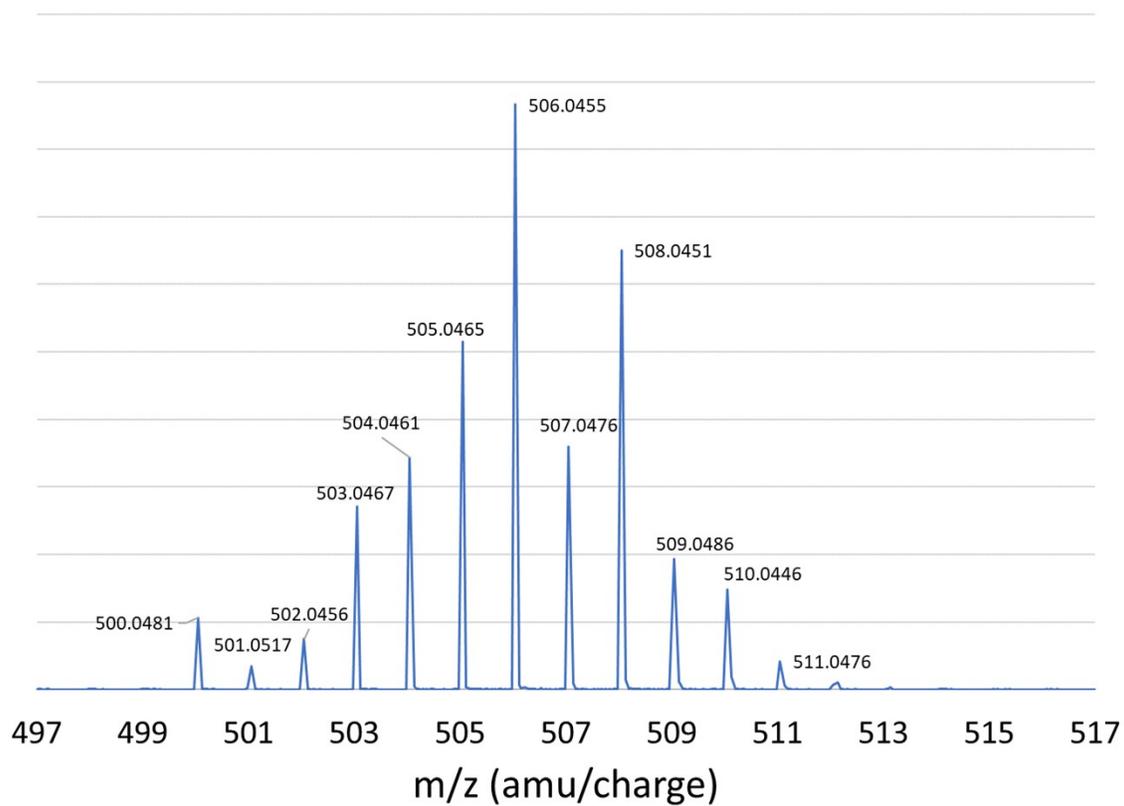


Figure S4. Observed (top) and calculated (bottom) isotope ratios for 1 in methanol.

Table S1. Overall conversion and oxidized product yields for THF oxidation by **1[Cl]** under various reaction conditions.^a

Conditions ^b	Yield ^c γ -Butyrolactone	Yield ^c Succinic Acid	Remaining Starting Material ^d
Air and Light	25.8%	3.7%	59%
Air and Dark	20.5%	2.8%	27.3%
N ₂ and Light	22%	2.7%	76.5%
N ₂ and Dark	22.8%	3.8%	47%

^aReaction conditions: 4.7 μ mol **1** (0.95% catalyst loading), 2.4 mmol CAN, 493 μ mol THF in 10 mL D₂O containing 19 μ mol 3-(trimethylsilyl)propionic-2,2,3,3-d₄ acid sodium salt as an internal standard at 20° C for 1 hr. ^bReaction run sealed using a septum either under air or nitrogen atmosphere, and with or without exclusion of light. ^cAs determined by ¹H NMR, mol product/initial mol THF. ^dAs determined by ¹H NMR, mol THF/initial mol THF.