

Supporting Information

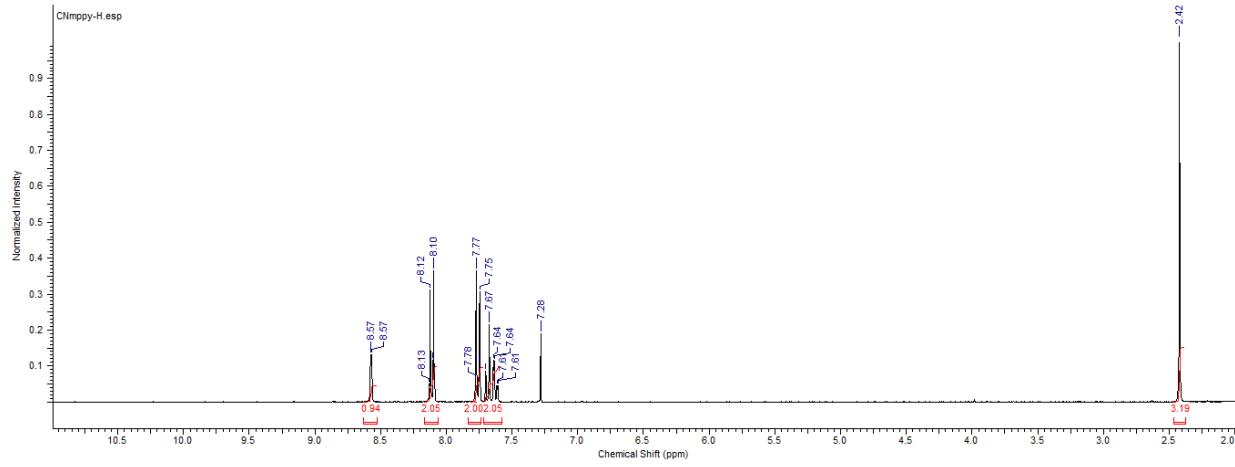
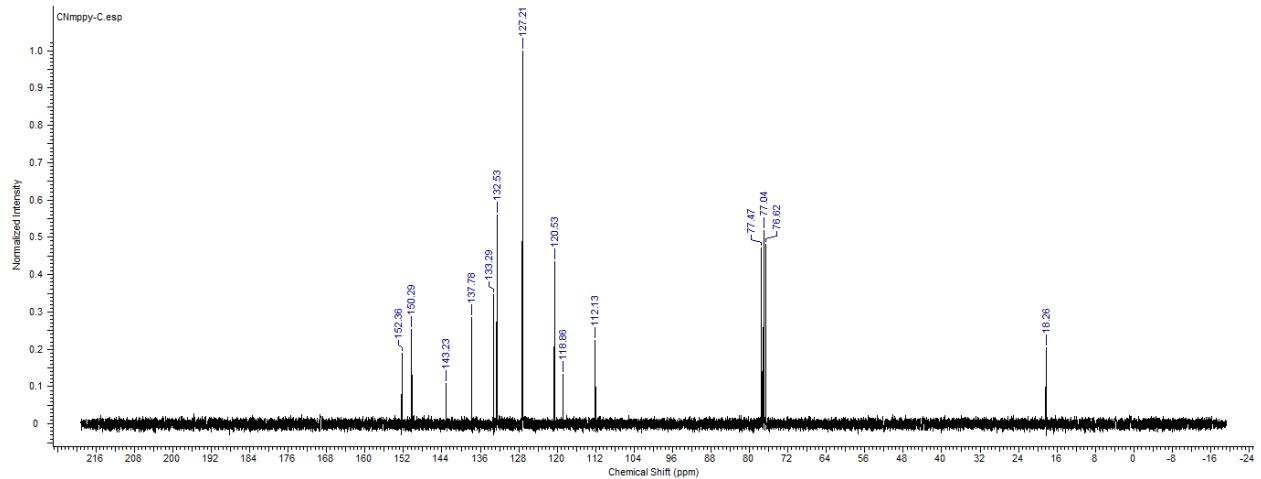
Cyano-decorated Ligands: A Powerful Alternative to Fluorination for Tuning the Photochemical Properties of Cyclometalated Ir(III) Complexes

Isaac N. Mills, Husain N. Kagalwala, Stefan Bernhard*

Department of Chemistry, Carnegie Mellon University, 4400 Fifth Avenue, Pittsburgh, PA 15213, United States

Table of Contents	Page
^1H -NMR, ^{13}C -NMR Data for Ligand 1	S2
^1H -NMR, ^{13}C -NMR Data for Complex 3a	S3
Cyclic Voltammogram of Complex 3a	S4
^1H -NMR, ^{13}C -NMR Data for Complex 3b	S4-S5
Cyclic Voltammogram of Complex 3b	S5

Supporting data for ligand 1

Figure S1: ^1H -NMR spectrum of **1** in CD_3Cl at 300 MHzFigure S2: ^{13}C -NMR spectrum of **1** in CD_3Cl at 75 MHz

Supporting data for $[\text{Ir}(\text{CNmppy})_2(\text{dtbbpy})]\text{PF}_6$, **3a**

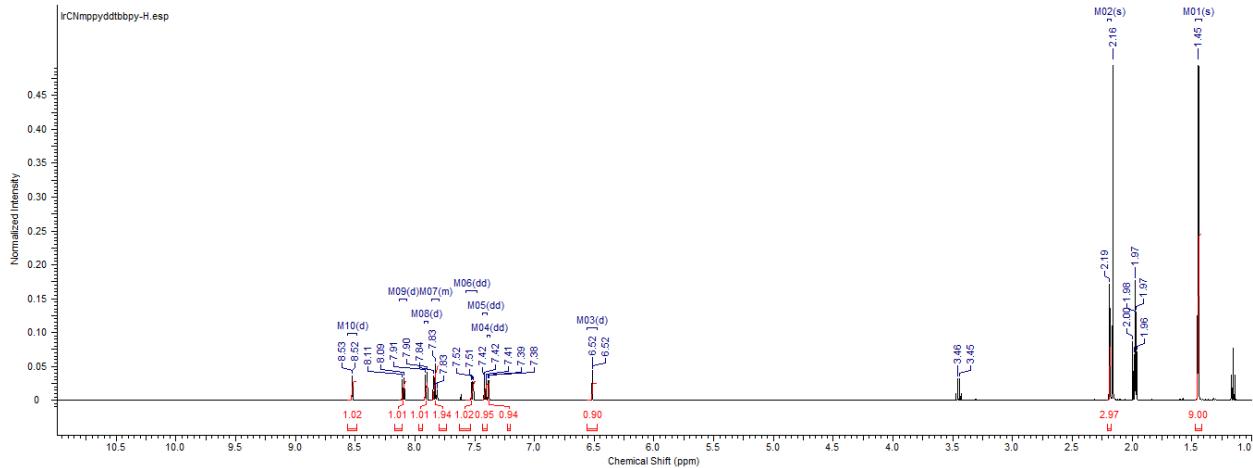


Figure S3: ^1H -NMR spectrum of **3a** in CD_3CN at 500 MHz

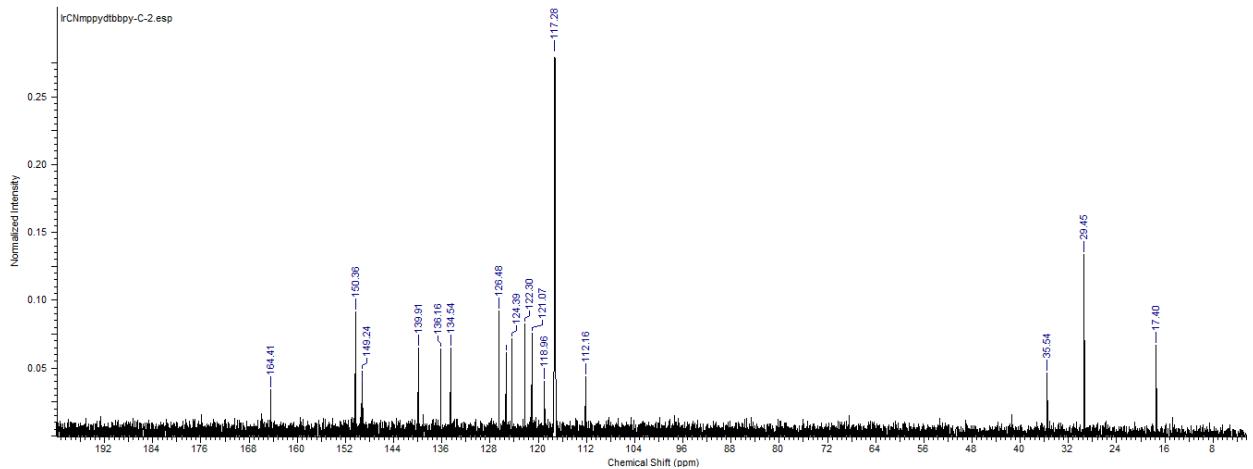


Figure S4: ^{13}C -NMR spectrum of **3a** in CD_3CN at 125 MHz

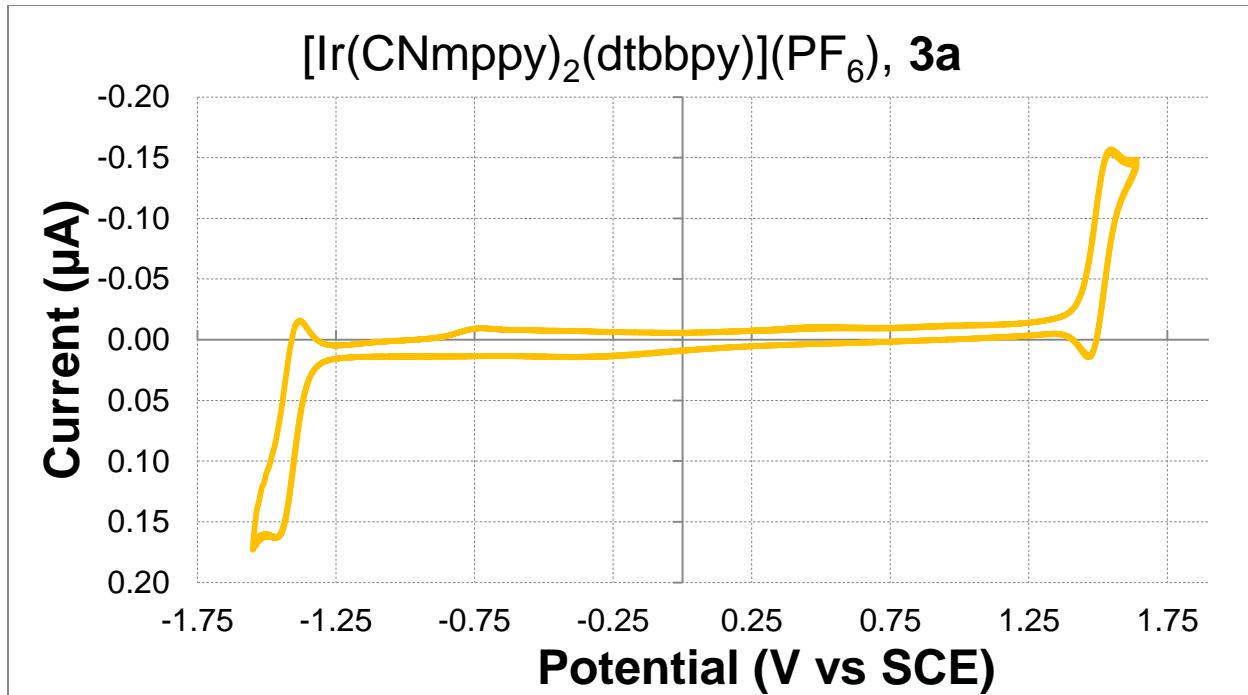


Figure S5: Cyclic voltammogram of **3a** in acetonitrile with 1 mM analyte and 0.1 M (tBu)₄NPF₆ as supporting electrolyte

Supporting data for [Ir(CNmppy)₂(dCNbpy)]PF₆, **3b**

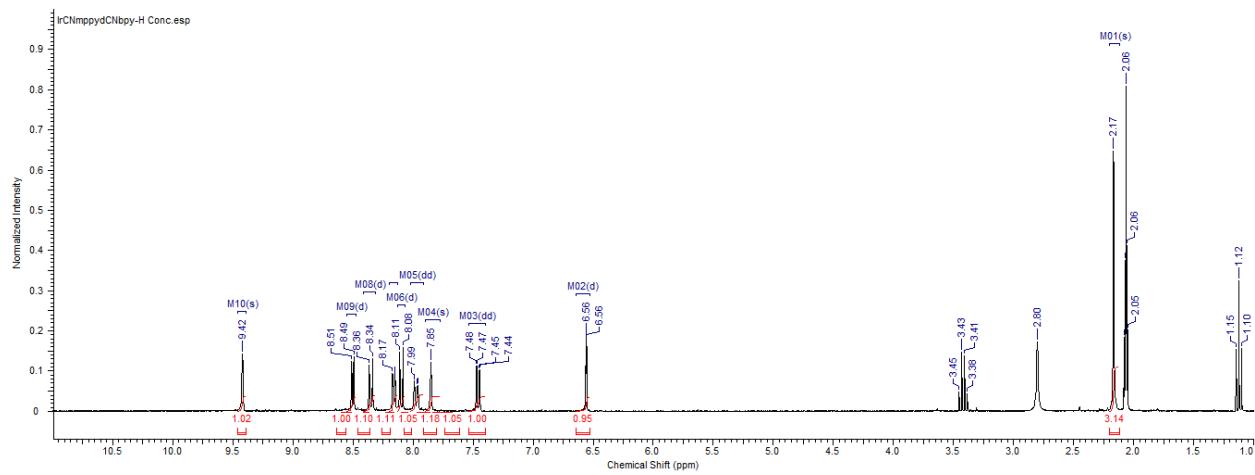


Figure S6: ¹H-NMR spectrum of **3b** in CD₃CN at 500 MHz

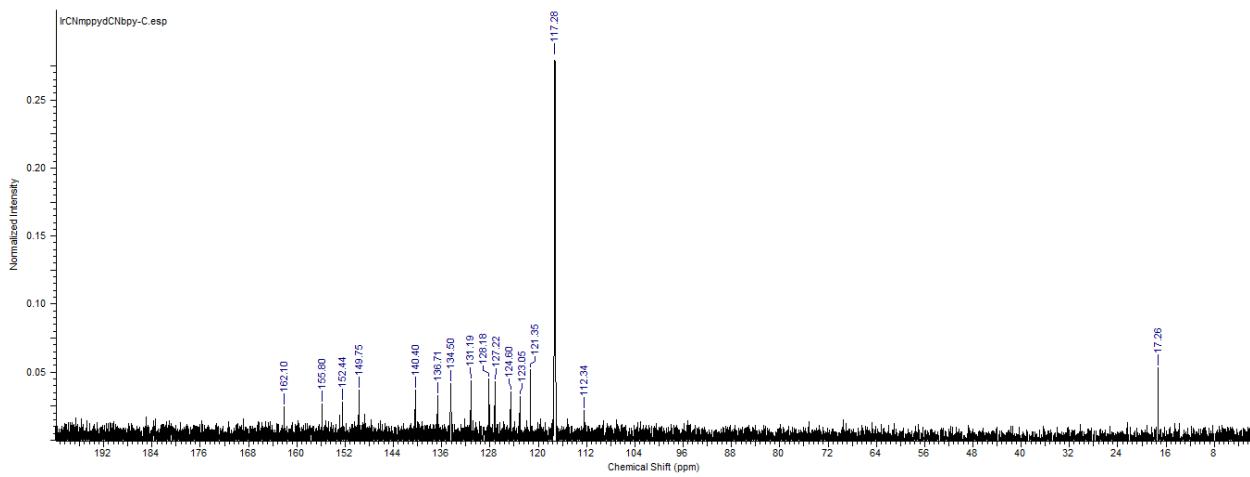


Figure S7: ^{13}C -NMR spectrum of **3b** in CD_3CN at 125 MHz

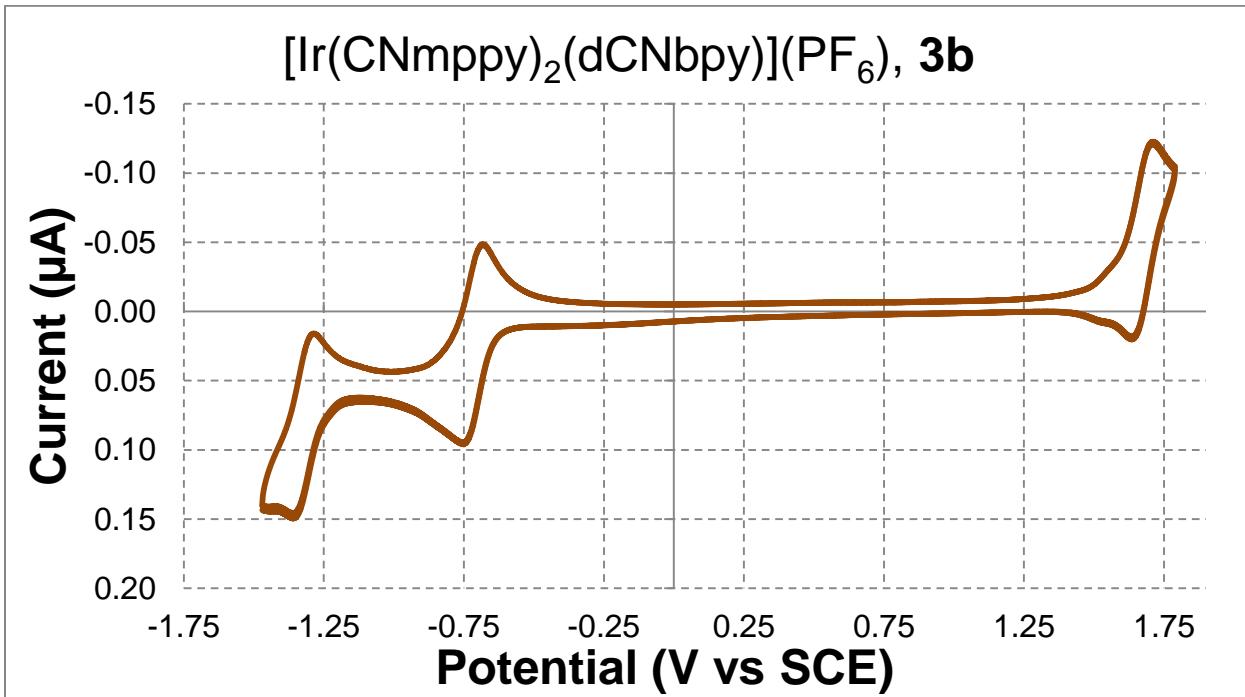


Figure S8: Cyclic voltammogram of **3b** in acetonitrile with 1 mM analyte and 0.1 M $(\text{tBu})_4\text{NPF}_6$ as supporting electrolyte