

Spectroscopic and Redox Properties of Amine-Functionalized $K_2[Os^{II}(bpy)(CN)_4]$ Complexes

Michael J. Ahrens,^{*a} Paul A. Bertin,^a Adam G. Gaustad,^a Dimitra Georganopoulou,^a Markus Wunder,^a
Gary F. Blackburn,^a Harry B. Gray,^b and Thomas J. Meade^{*c}

^aOhmx Corporation, 1801 Maple Avenue, Suite 6143, Evanston, Illinois 60201, USA. E-mail: michael@ohmx.com. Fax: 1-847-491-8510

^bArnold and Mabel Beckman Laboratories of Chemical Synthesis, California Institute of Technology, 1200 East California Blvd. MC 139-74, Pasadena, California, 91125, USA.

^cDepartments of Chemistry, Biochemistry and Molecular and Cell Biology, Neurobiology and Physiology, and Radiology, Northwestern University, 2145 Sheridan Road, Evanston, Illinois 60208, USA. E-mail: tmeade@northwestern.edu

Electronic spectra for complexes 1–6.....	2
Molar absorptivity data for complexes 1–6.....	2
Cyclic voltammetry data for complexes 1–6.....	3
$K_2[Os(CN)_4-5\text{-aminoethyl-}5'\text{-methyl-}2,2'\text{-bipyridine}]$ NMR characterization data.....	4
$K_2[Os(CN)_4-5,5'\text{-dimethyl-}2,2'\text{-bipyridine}]$ NMR characterization data.....	5
$K_2[Os(CN)_4-5,5'\text{-bis(aminomethyl)-}2,2'\text{-bipyridine}]$ NMR characterization data.....	6
$K_2[Os(CN)_4-4\text{-aminoethyl-}4'\text{-methyl-}2,2'\text{-bipyridine}]$ NMR characterization data.....	7
$K_2[Os(CN)_4-4,4'\text{-dimethyl-}2,2'\text{-bipyridine}]$ NMR characterization data.....	8
$K_2[Os(CN)_4-4,4'\text{-bis(aminomethyl)-}2,2'\text{-bipyridine}]$ NMR characterization data.....	9

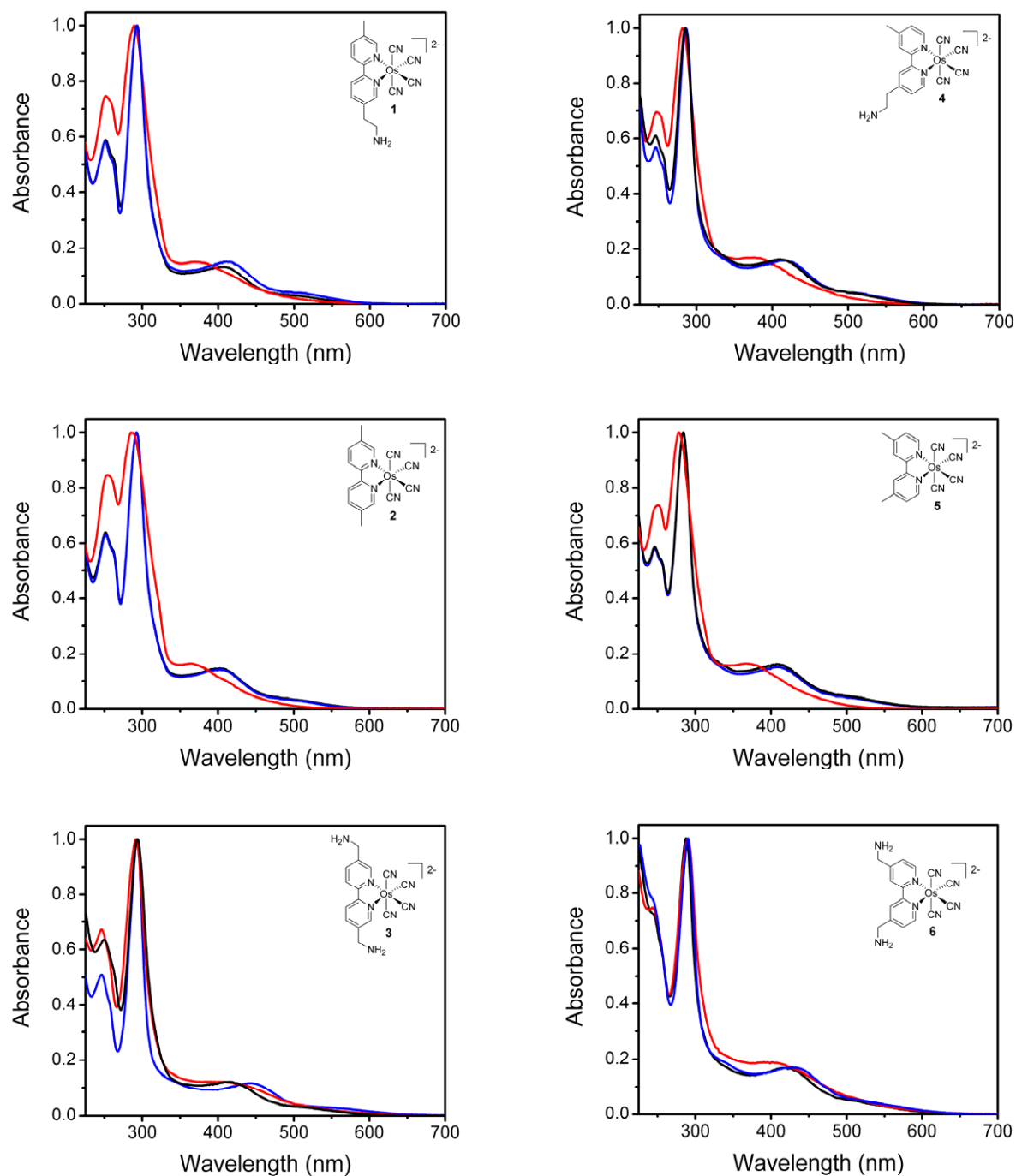


Figure S1 Electronic spectra for complexes 1–6 in water at pH = 1.5 (—), 5.5 (—), and 12 (—).

Table S1 Molar absorptivities ($\times 10^{-3}$) for complexes 1–6.

complex	λ_{IL} (cm^{-1})	ϵ ($\text{M}^{-1} \text{cm}^{-1}$)	λ_{MLCT} (cm^{-1})	ϵ ($\text{M}^{-1} \text{cm}^{-1}$)
1	294	19.5	408	3.1
2	294	23.0	404	3.5
3	294	23.5	414	3.3
4	286	19.6	409	3.2
5	285	20.6	410	3.1
6	292	19.6	418	3.1

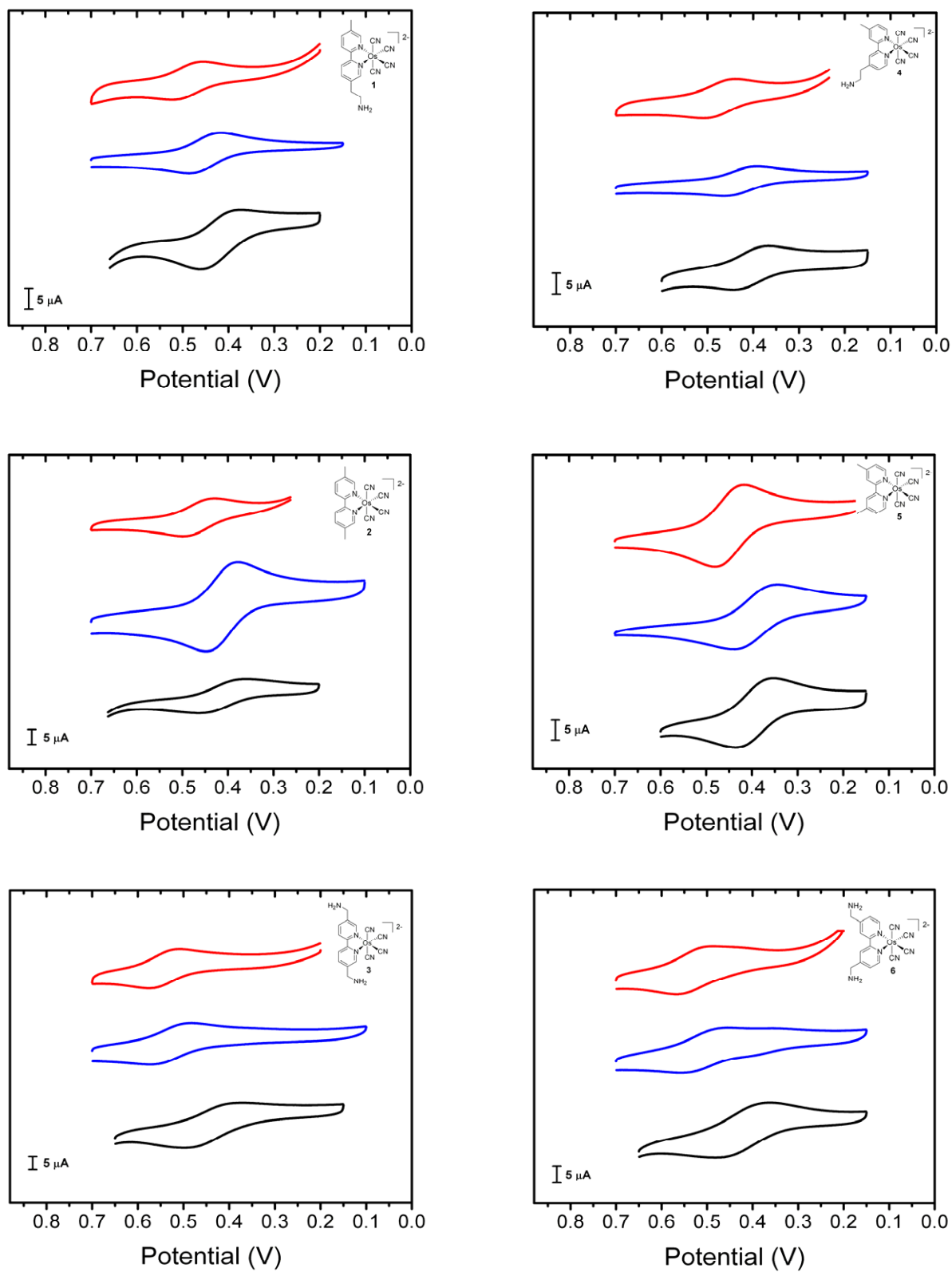
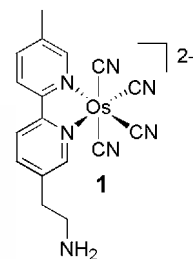
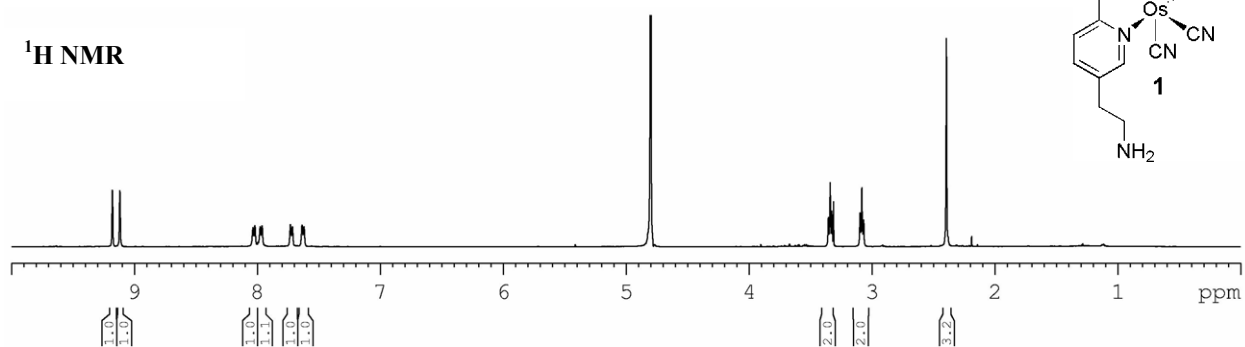


Figure S2 Cyclic voltammograms for complexes 1–6 in 0.1 M KCl at pH = 1.5 (→), 5.5 (→), and 12 (→).

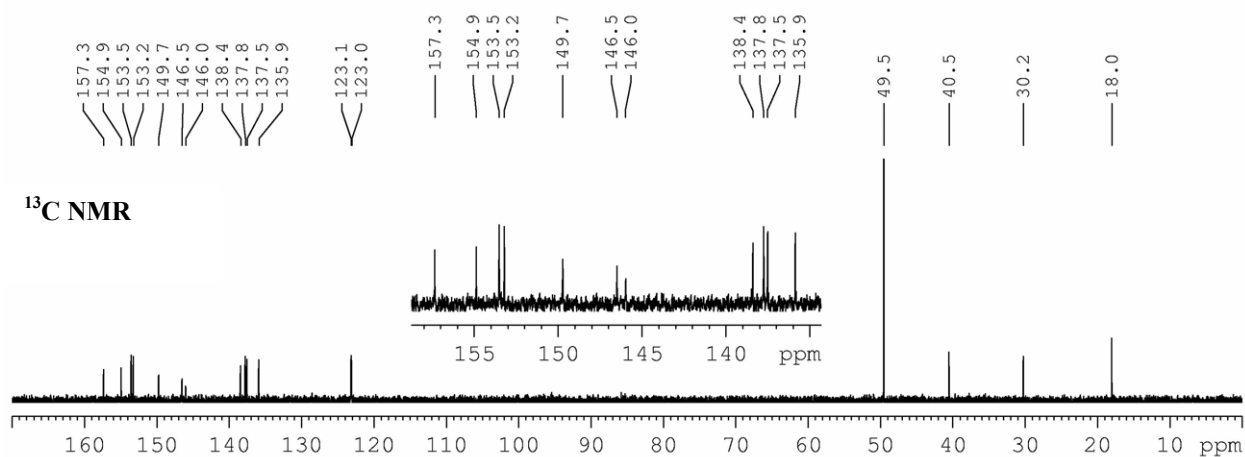
Ohm γ TM



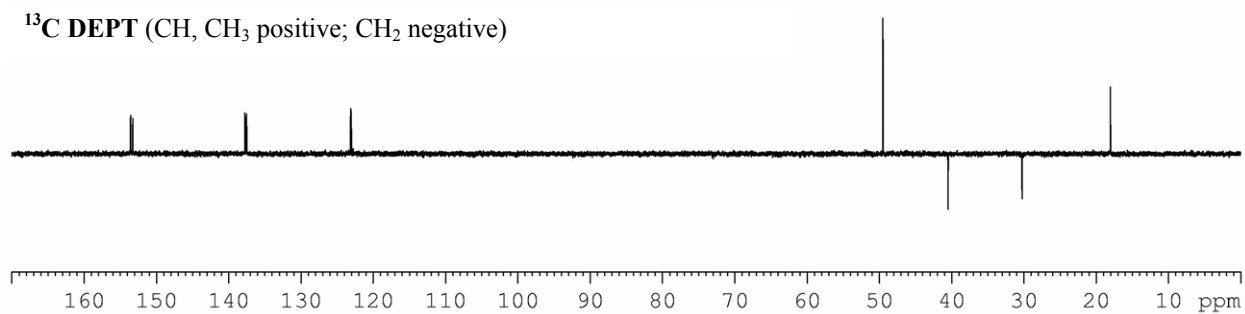
¹H NMR



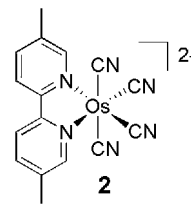
¹³C NMR



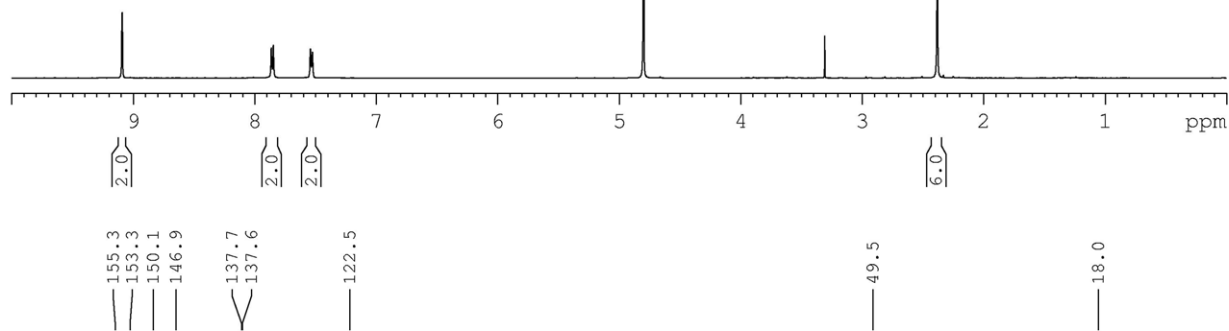
¹³C DEPT (CH, CH₃ positive; CH₂ negative)



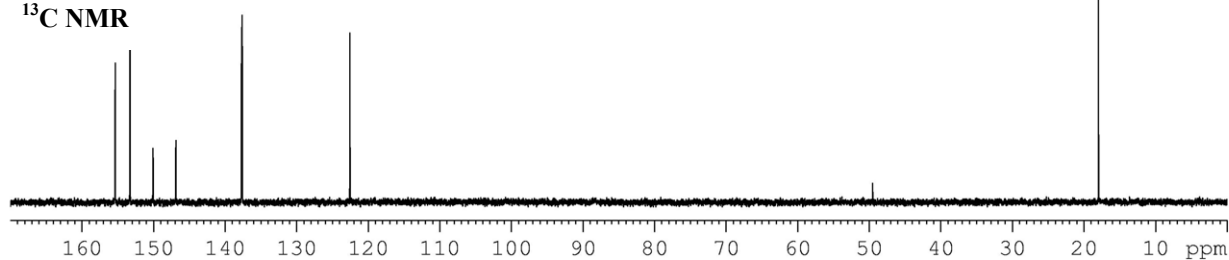
Ohm[®]



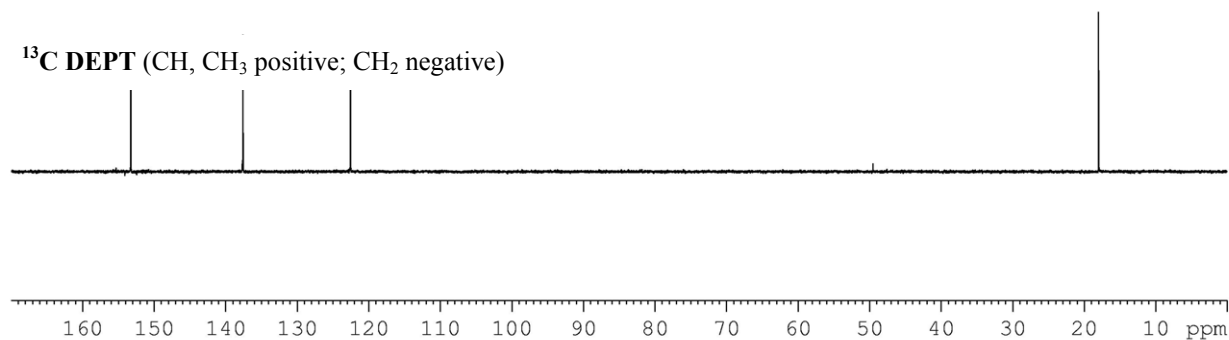
¹H NMR

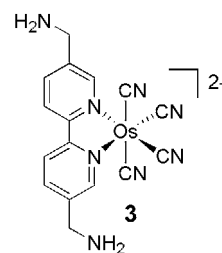


¹³C NMR

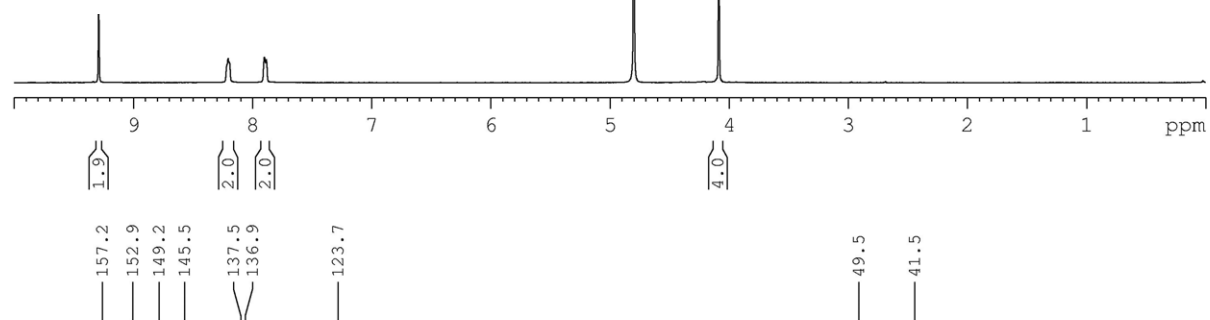


¹³C DEPT (CH, CH₃ positive; CH₂ negative)

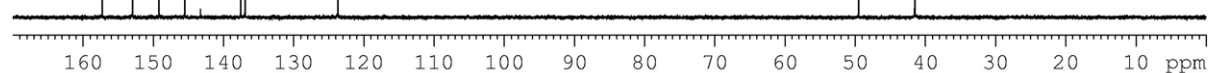




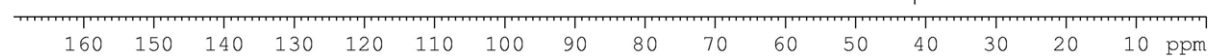
¹H NMR

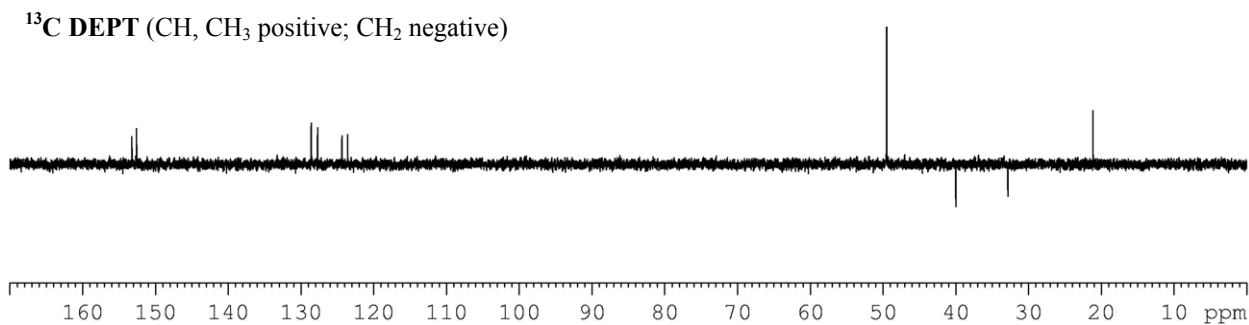
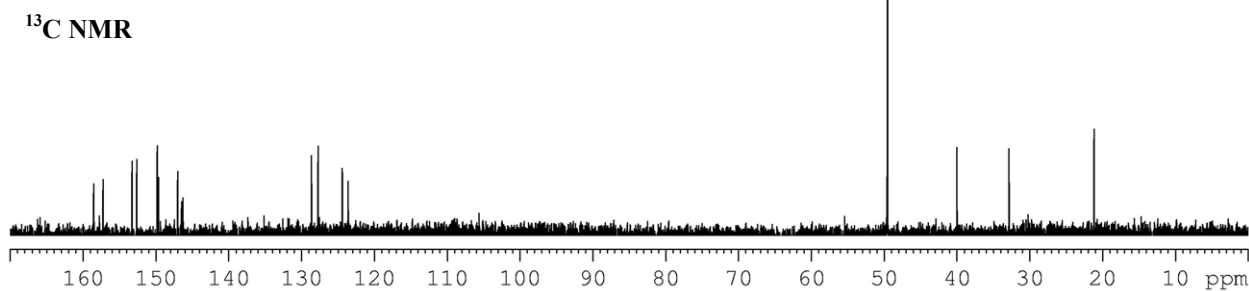
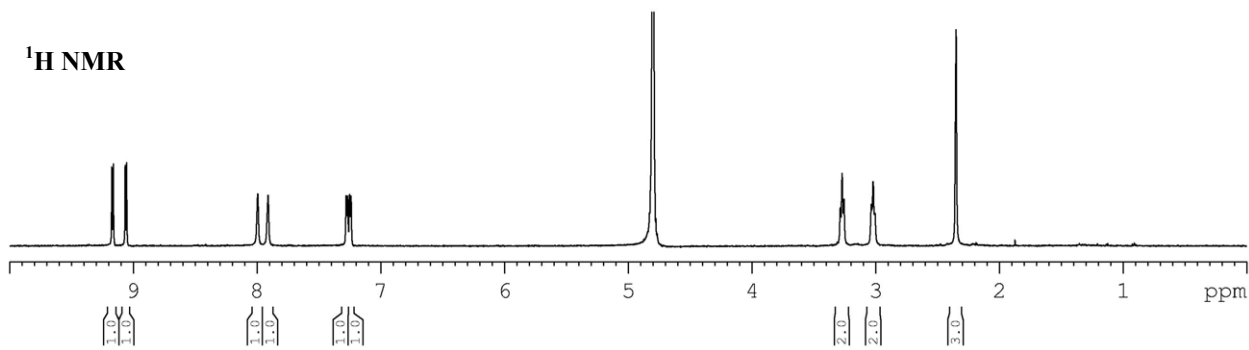
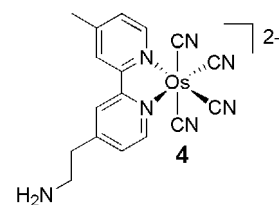


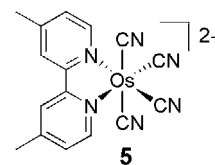
¹³C NMR



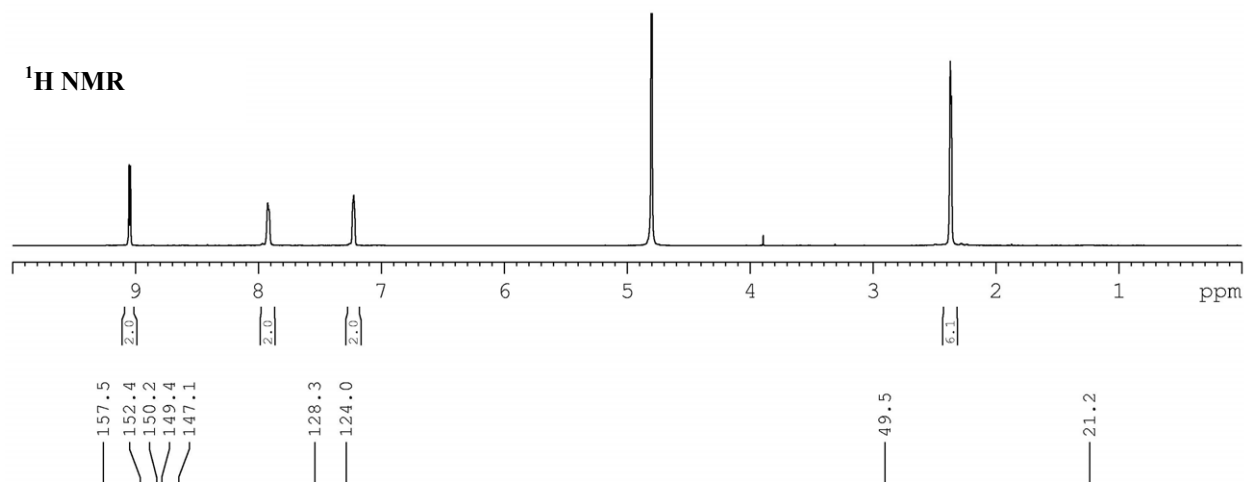
¹³C DEPT (CH, CH₃ positive; CH₂ negative)



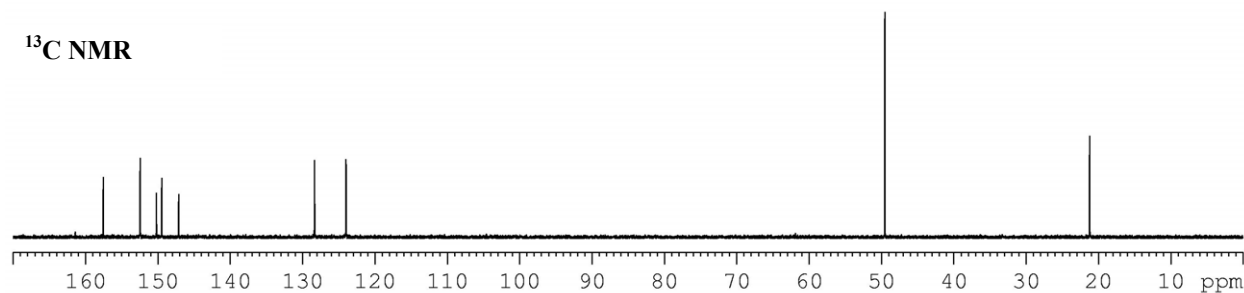




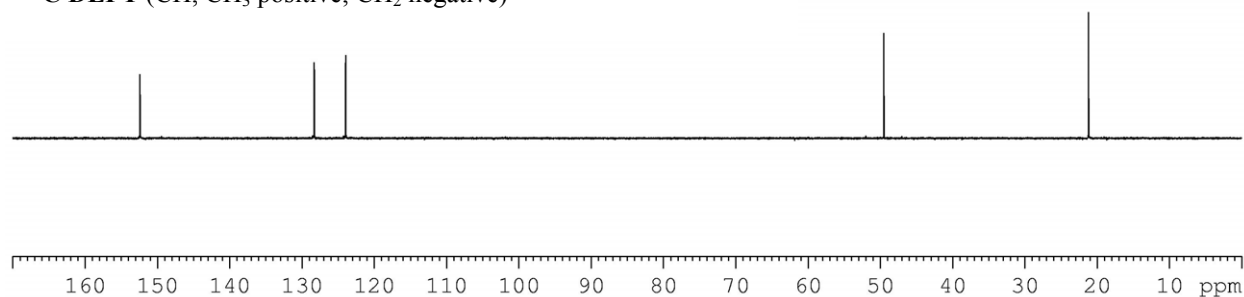
¹H NMR

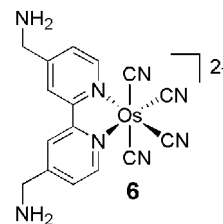


¹³C NMR

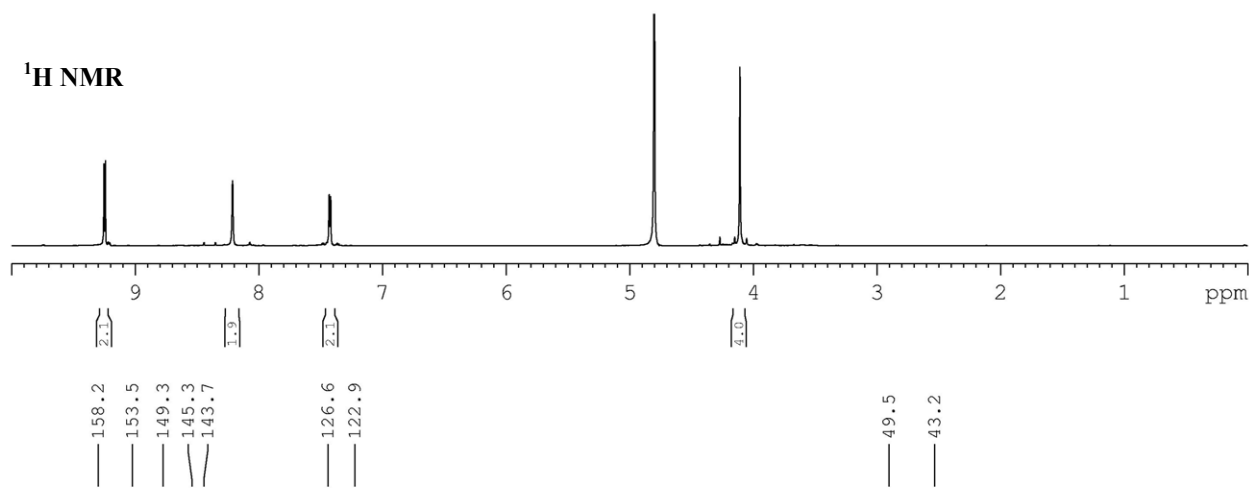


¹³C DEPT (CH, CH₃ positive; CH₂ negative)

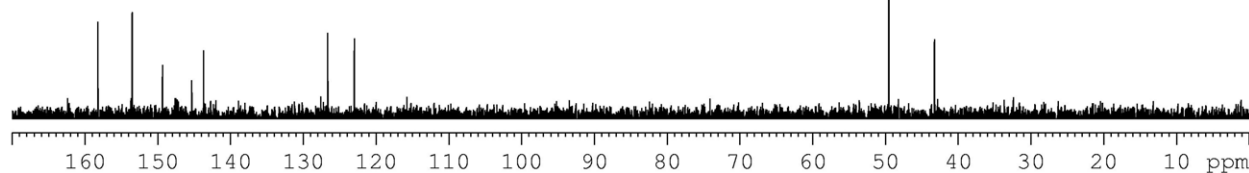




¹H NMR



¹³C NMR



¹³C DEPT (CH, CH₃ positive; CH₂ negative)

