

Copper(II) complexes derived from naphthalene-based halogenated Schiff bases: Synthesis, structural analysis, DFT computational studies and *in vitro* biological activities

Segun D. Oladipo,^{a,b*} Robert C. Luckay,^{a*}

^aDepartment of Chemistry and Polymer Science, Stellenbosch University, Private Bag X1, Matieland 7602, South Africa

^bDepartment of Chemical Sciences, Olabisi Onabanjo University, P.M.B 2002, Ago-Iwoye, Nigeria.

*Corresponding authors: Dr S. D. Oladipo (segun.oladipo@oouagoiwoye.edu.ng) and Prof. R.C. Luckay (rluckay@sun.ac.za)

Supplementary information

Table of contents

Figures	Page
Figure S1: FT-IR spectrum for L1	2
Figure S2: FT-IR spectrum for L2	3
Figure S3: FT-IR spectrum for 1	4
Figure S4: FT-IR spectrum for 2	5
Figure S5: ¹ H-NMR spectrum for L1	6
Figure S6: ¹³ C-NMR spectrum for L1	7
Figure S7: ¹ H-NMR spectrum for L2	8
Figure S8: ¹³ C-NMR spectrum for L2	9
Figure S9: EPR spectrum for 2	9
Figure S10: EPR spectrum for 1	10
Figure S11: Mass spectrum for L1	10
Figure S12: Mass spectrum for L2	11
Figure S13: Mass spectrum for 1	11
Figure S14: Mass spectrum for 2	12
Figure S15: Optimized structures for L1 , L2 , 1 and 2	12
Figure S16: Electronic absorption spectra of 1 and 2 at high concentration	13

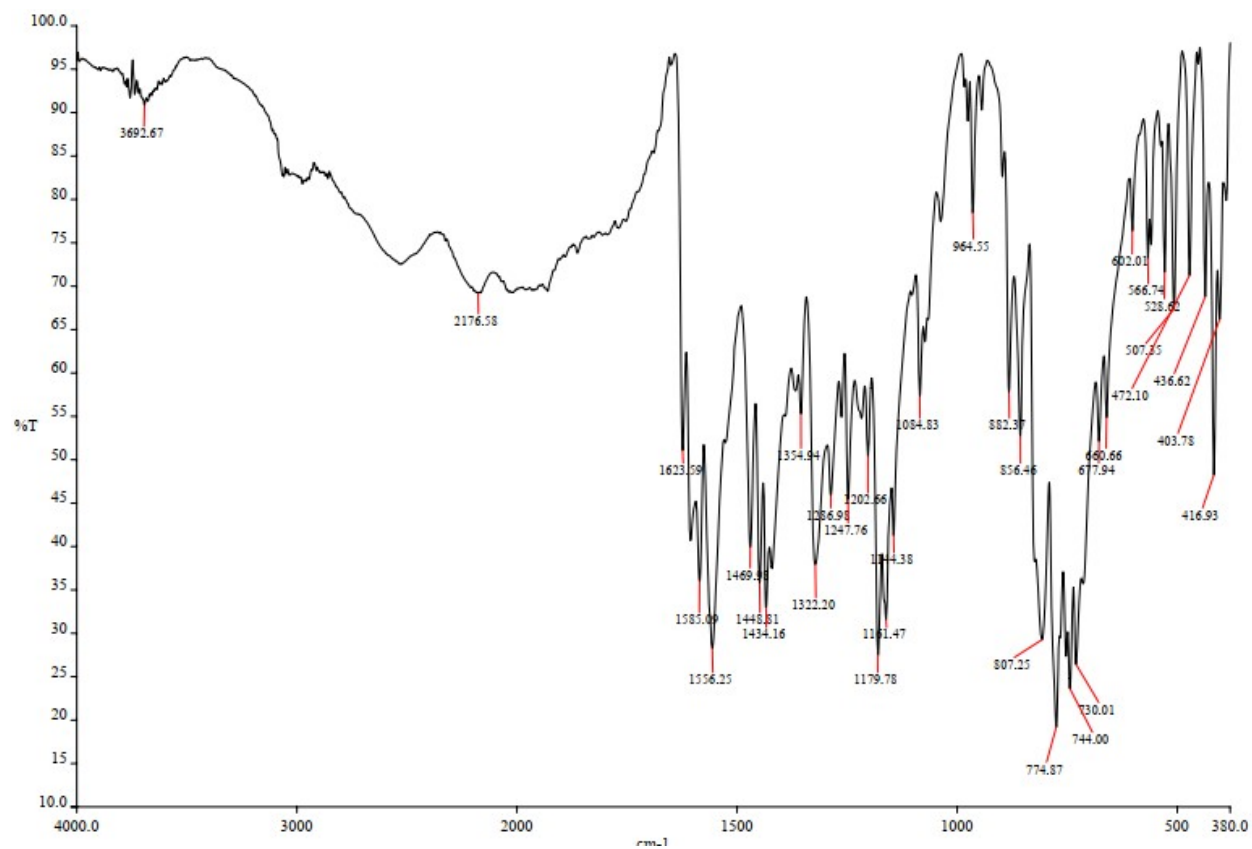


Figure S1: IR Spectrum of L1

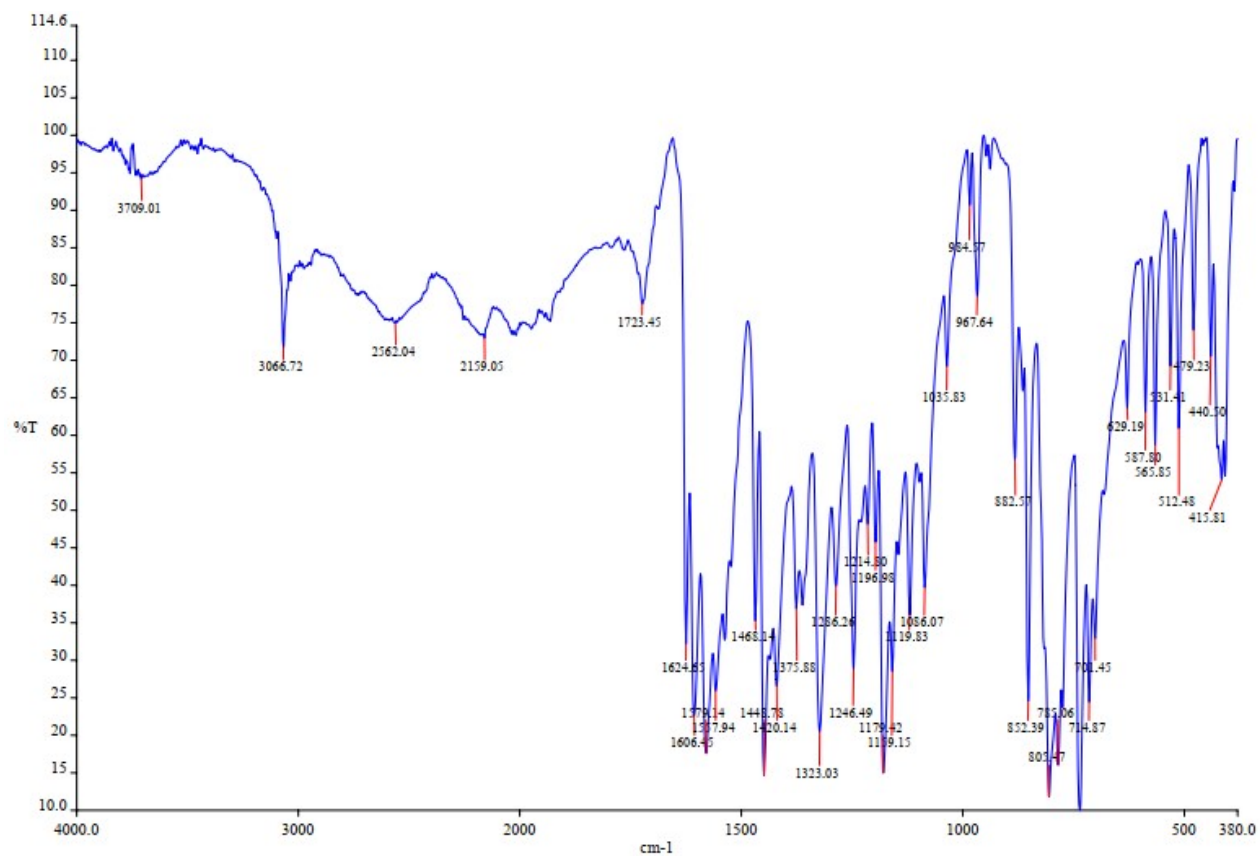


Figure S2: IR Spectrum of L2

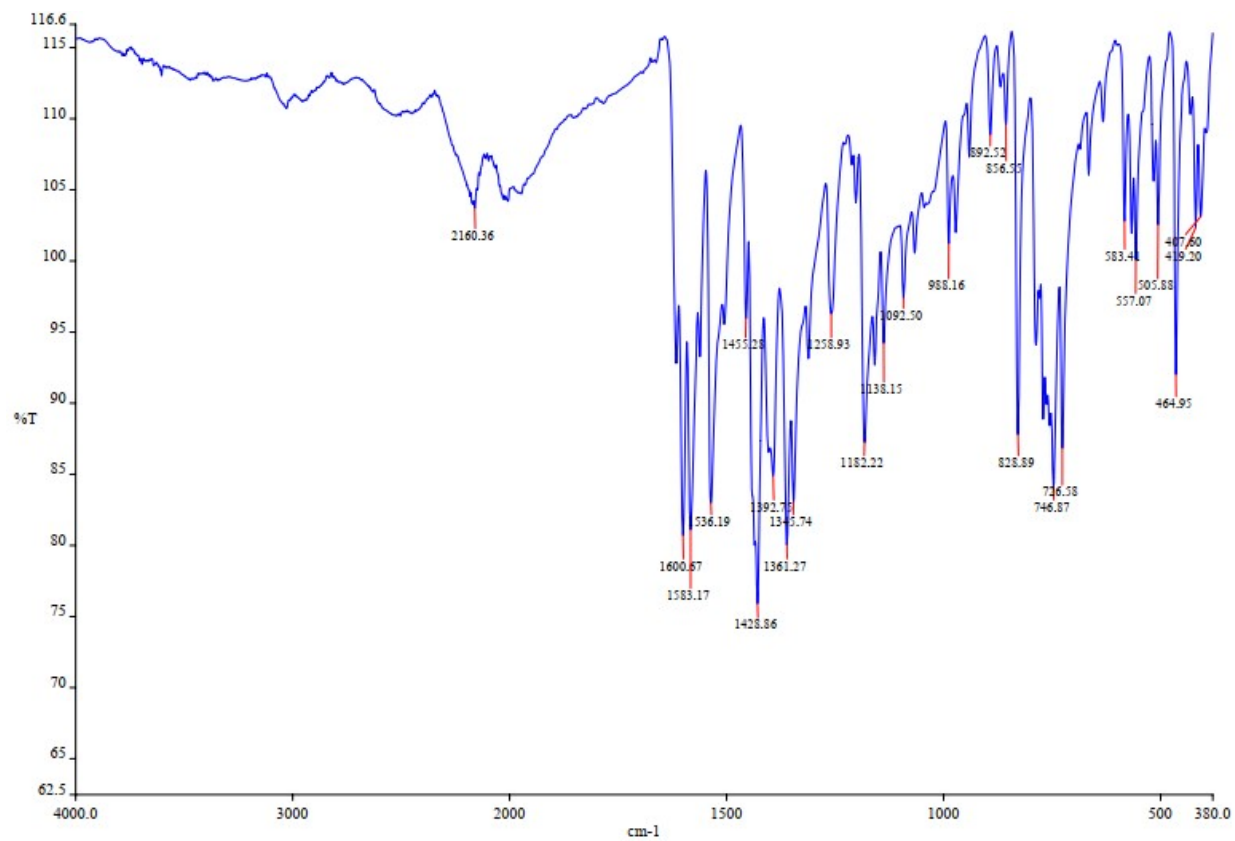


Figure S3: IR Spectrum of **1**

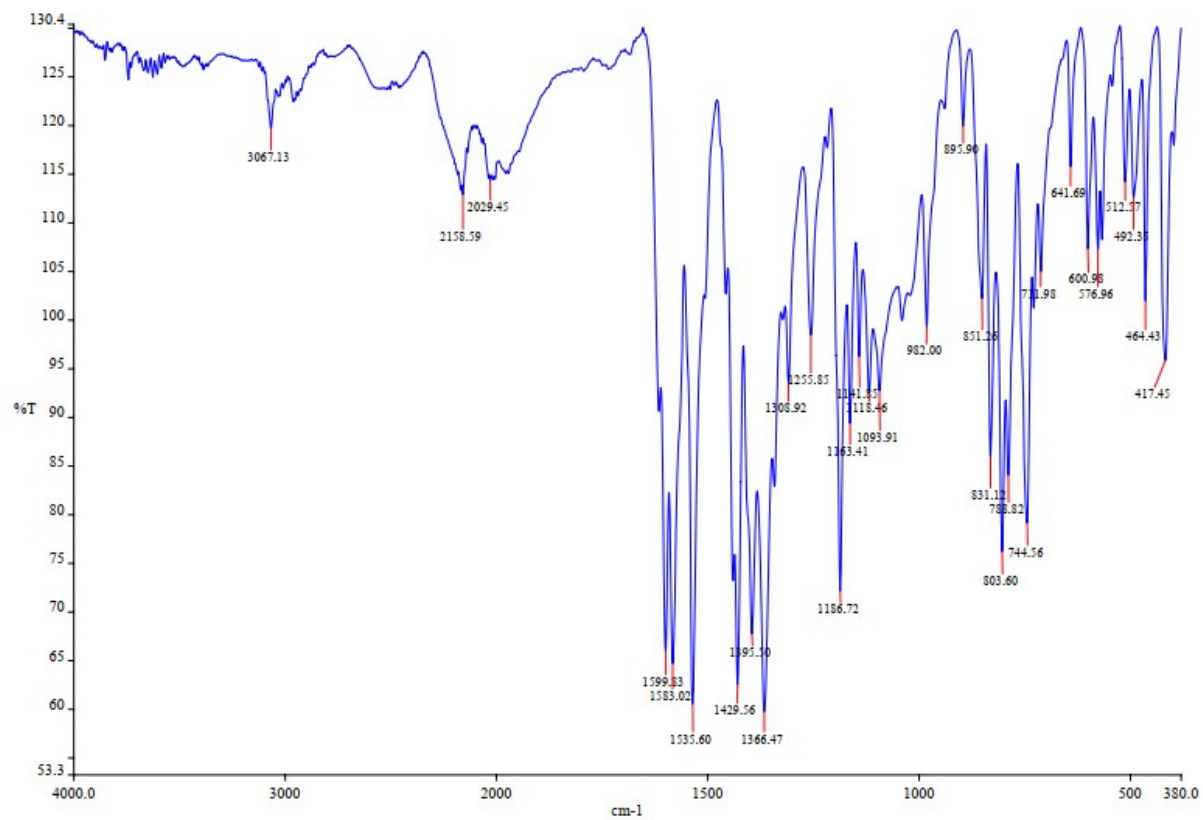


Figure S4: IR Spectrum of 2

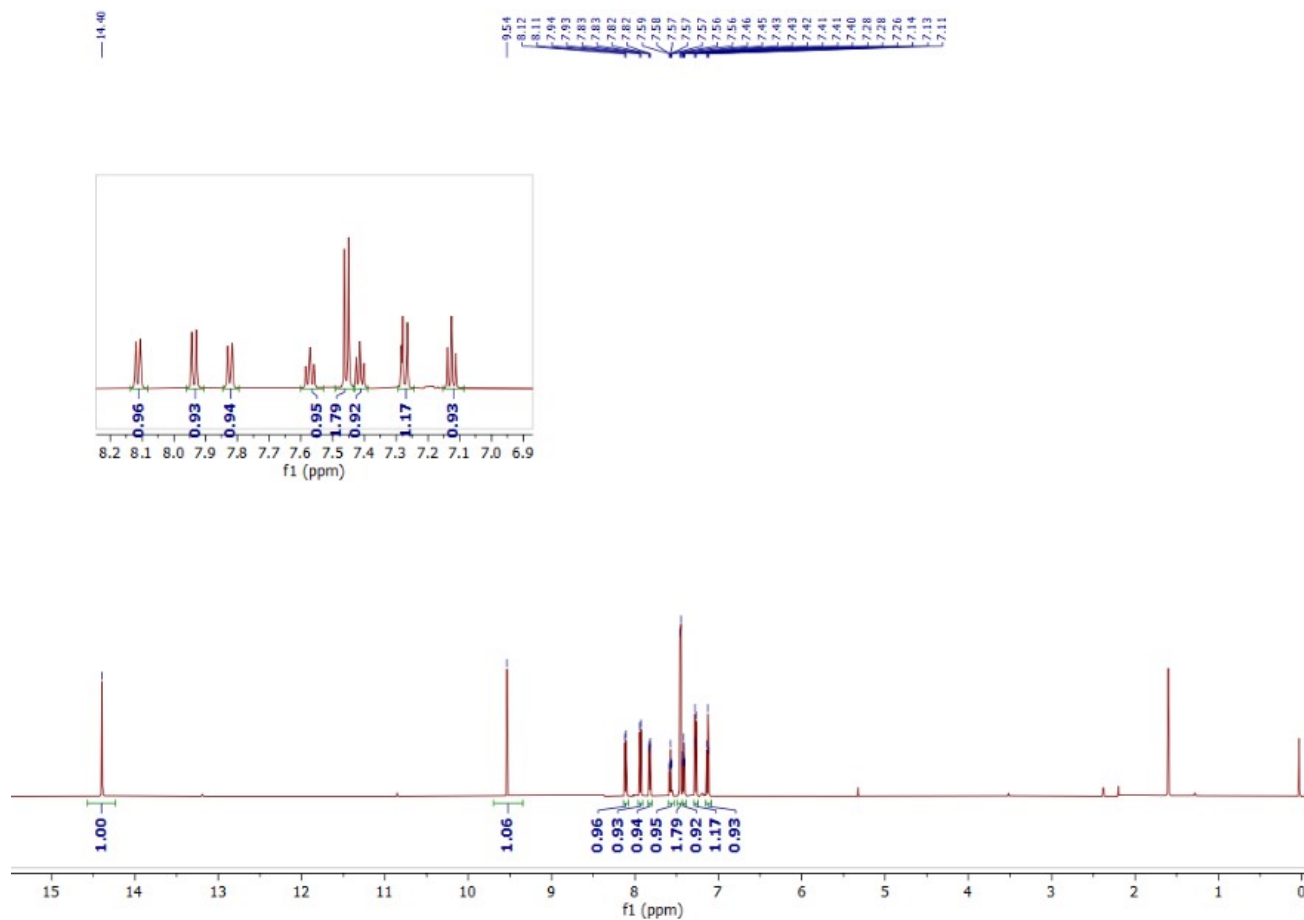


Figure S5: $^1\text{H-NMR}$ Spectrum of L1

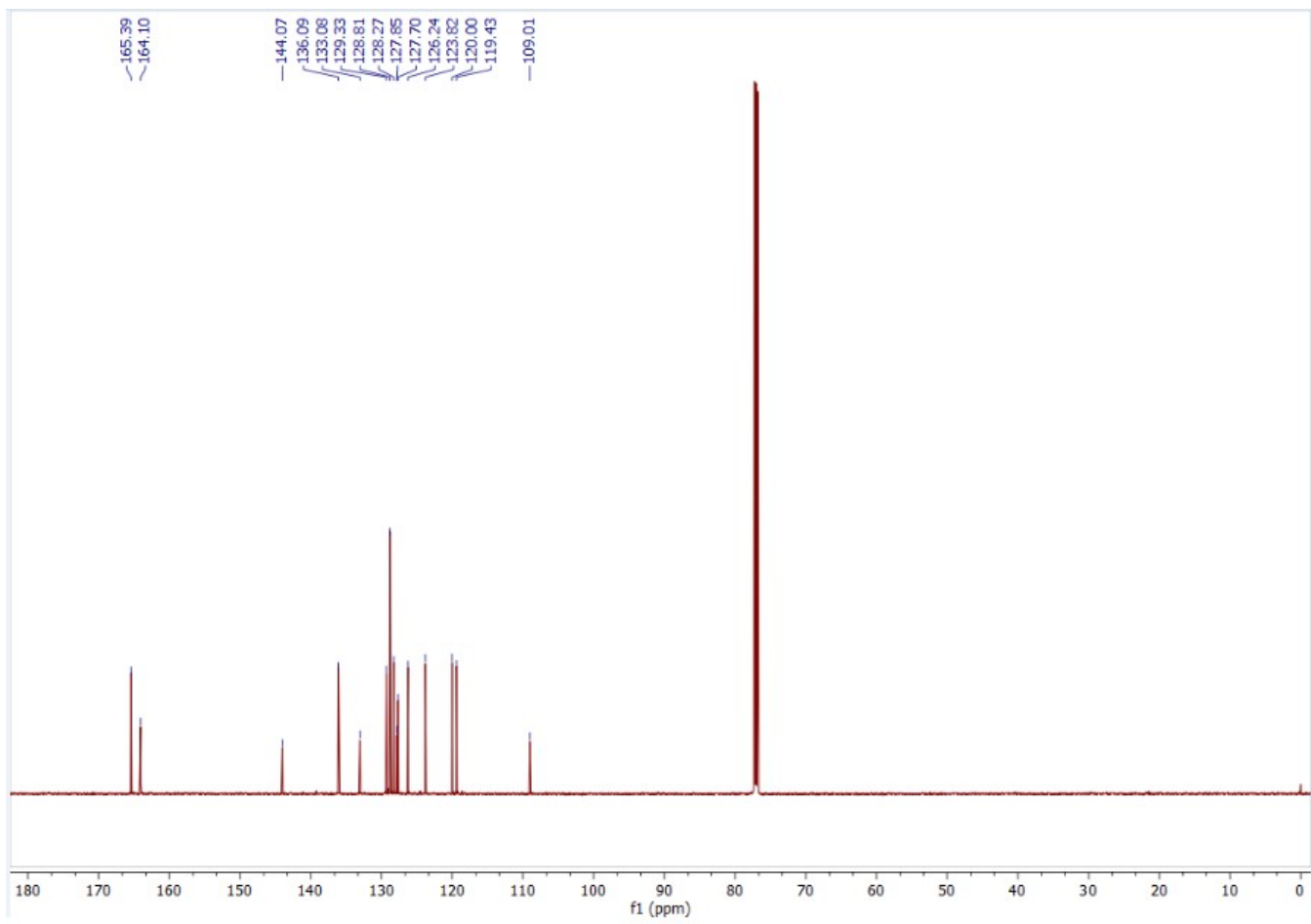


Figure S6: ^{13}C -NMR Spectrum of L1

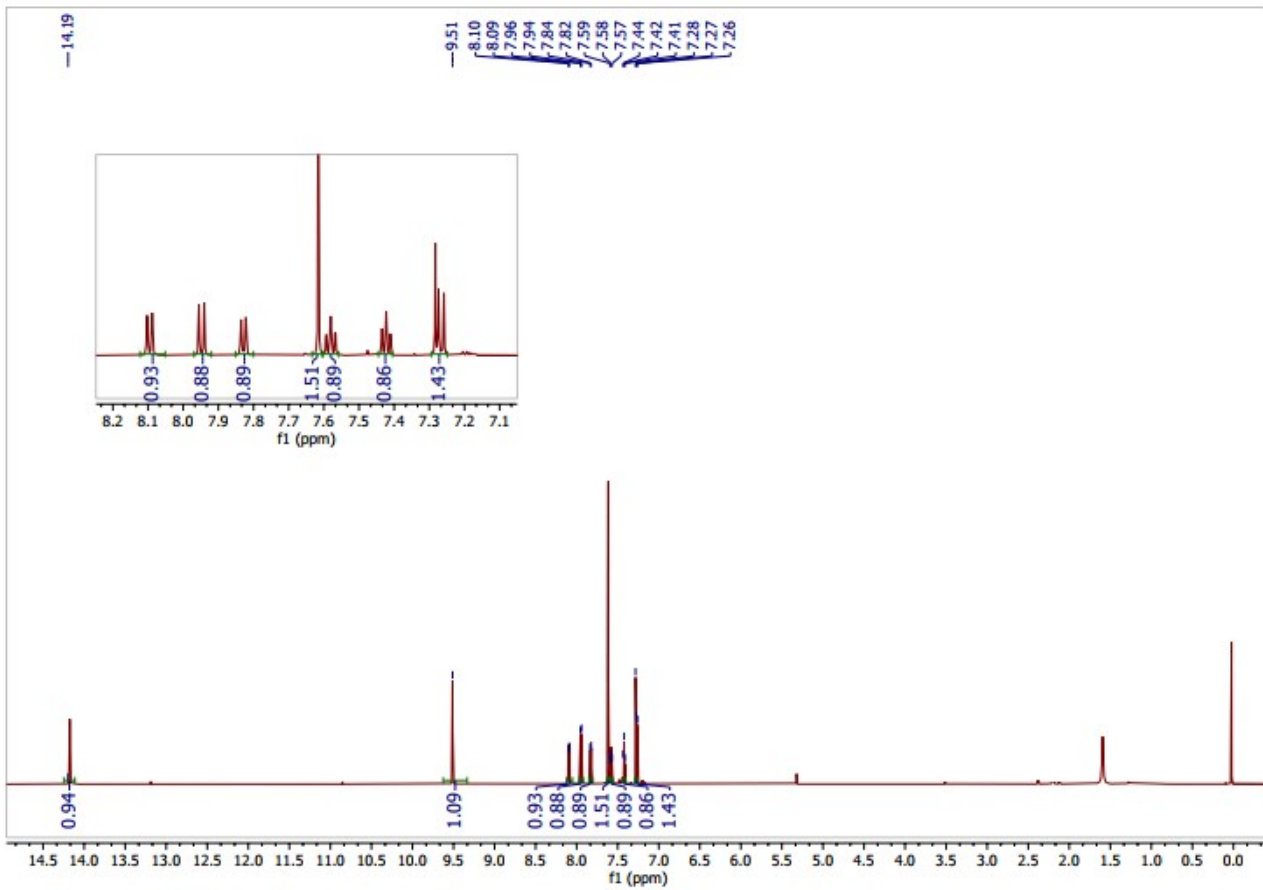


Figure S7: ¹H-NMR Spectrum of L2

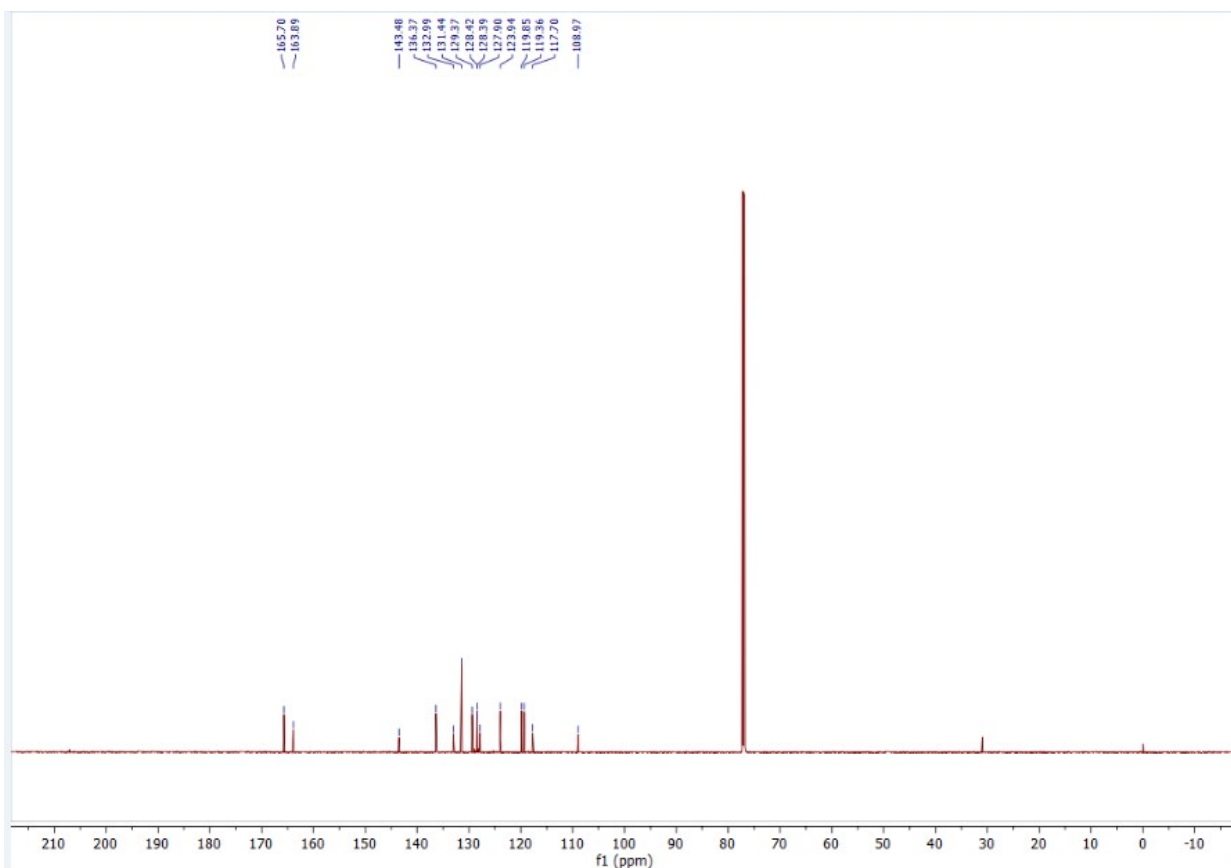


Figure S8: ^{13}C -NMR Spectrum of L2

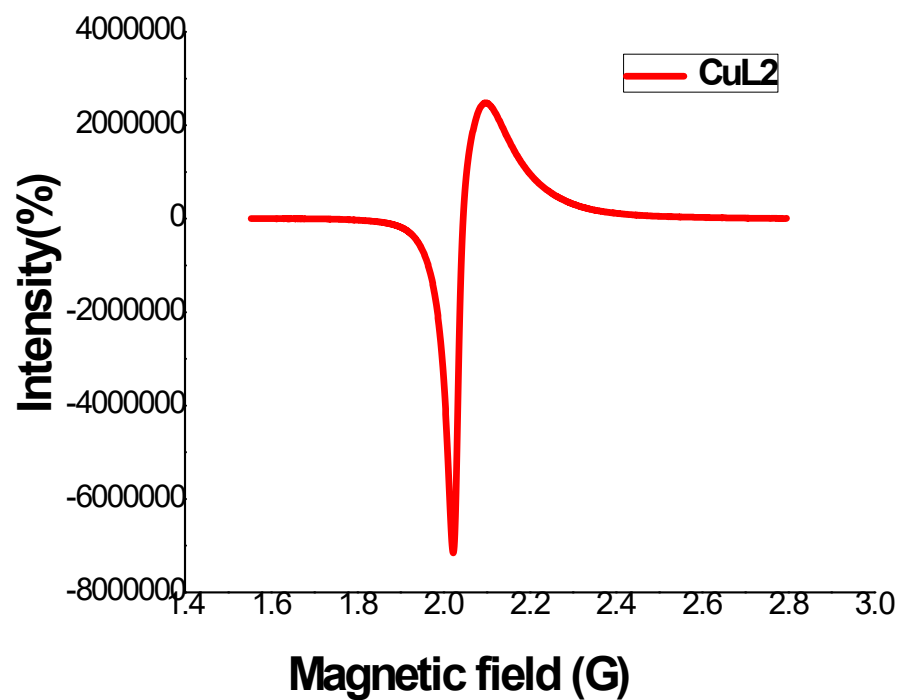


Figure S9: EPR of 2

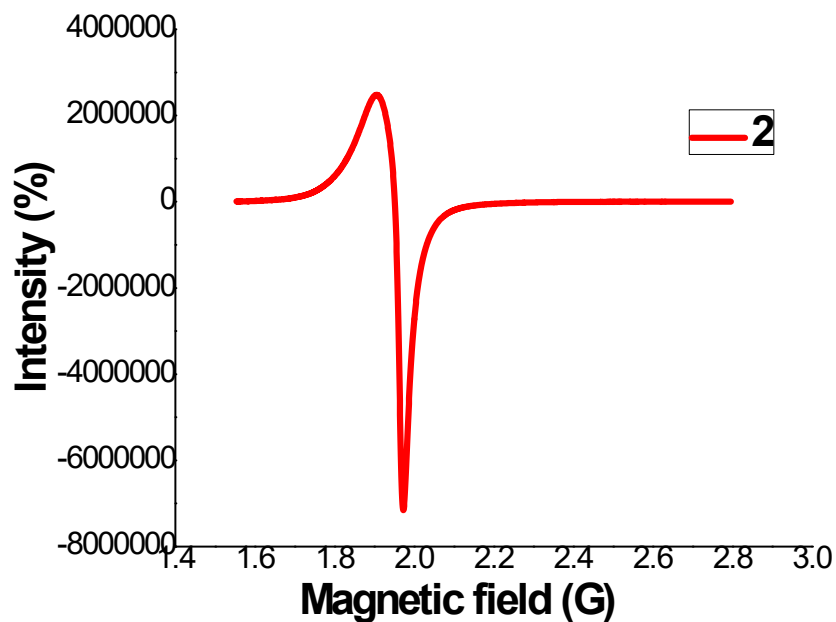


Figure S10: EPR of 1

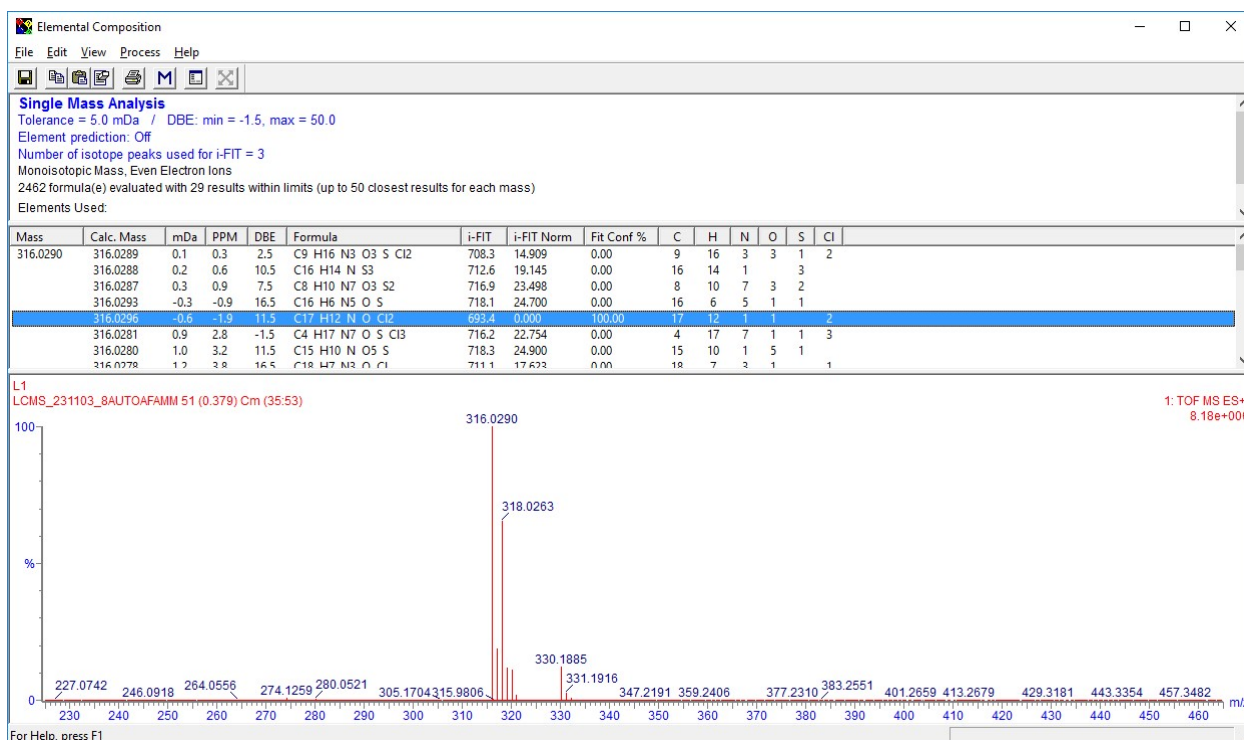


Figure S11: Mass spectrum for L1

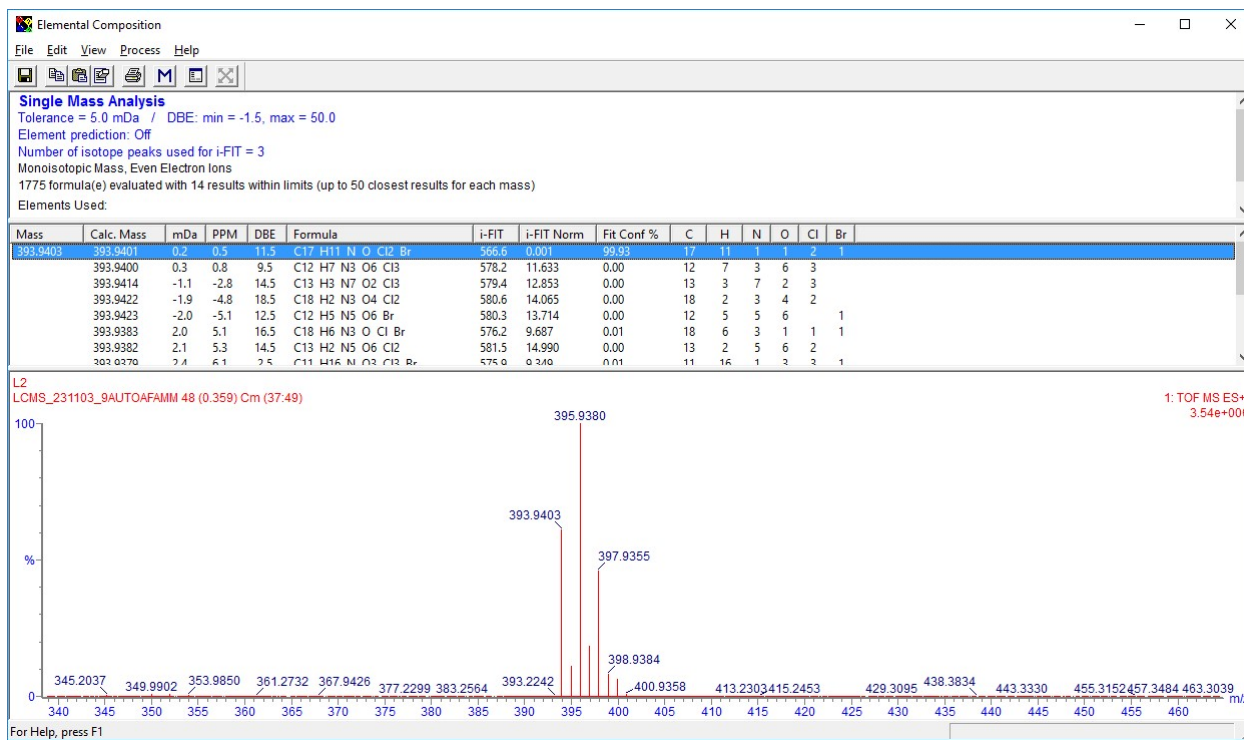


Figure S12: Mass spectrum for L2

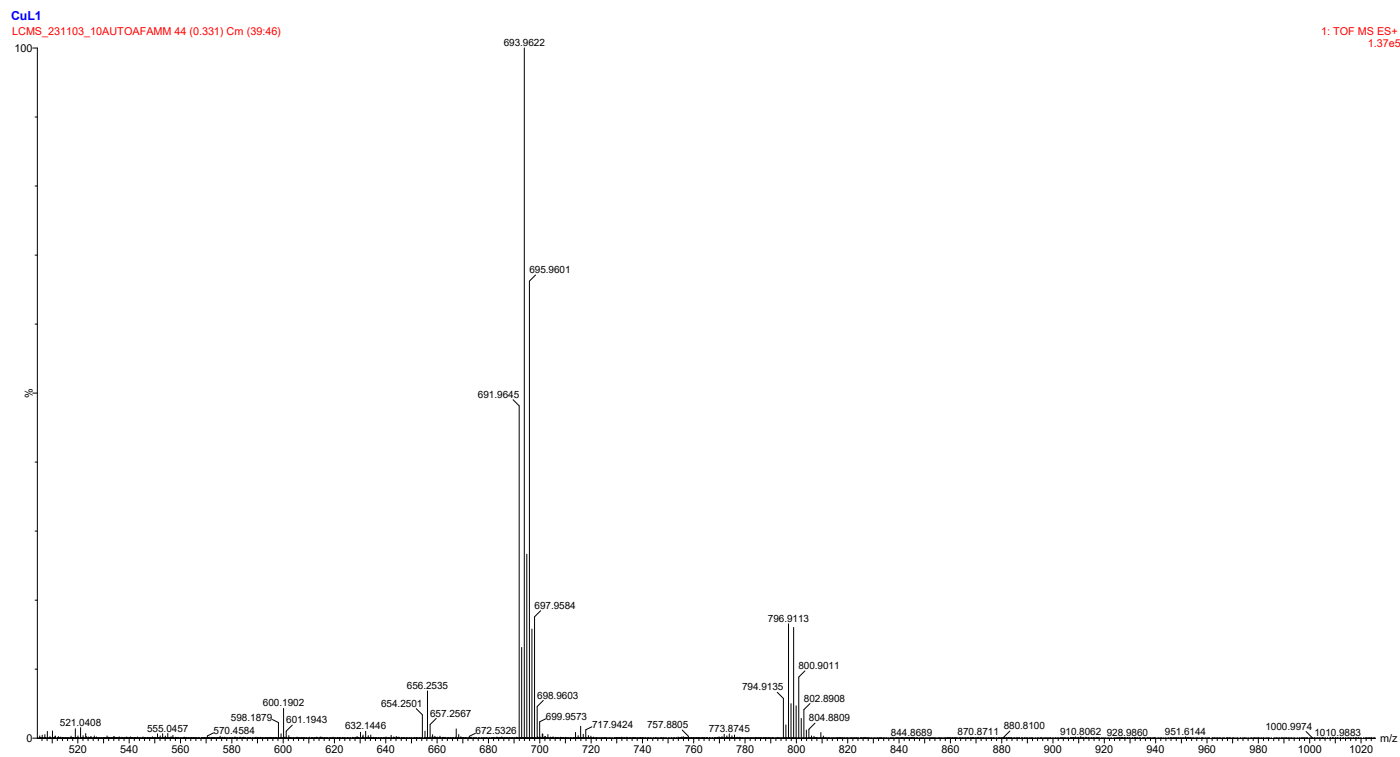


Figure S13: Mass spectrum for complex 1

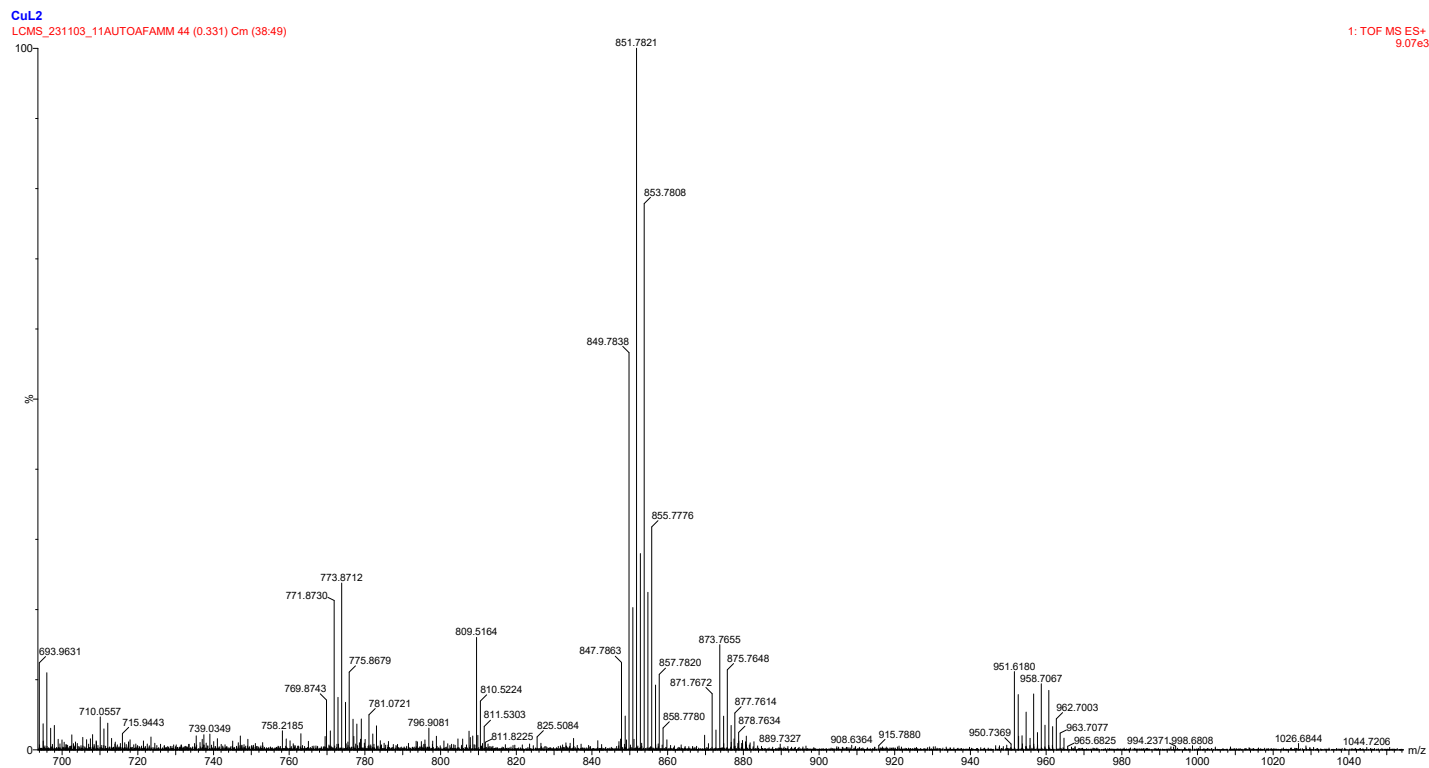


Figure S14: Mass spectrum for complex 2

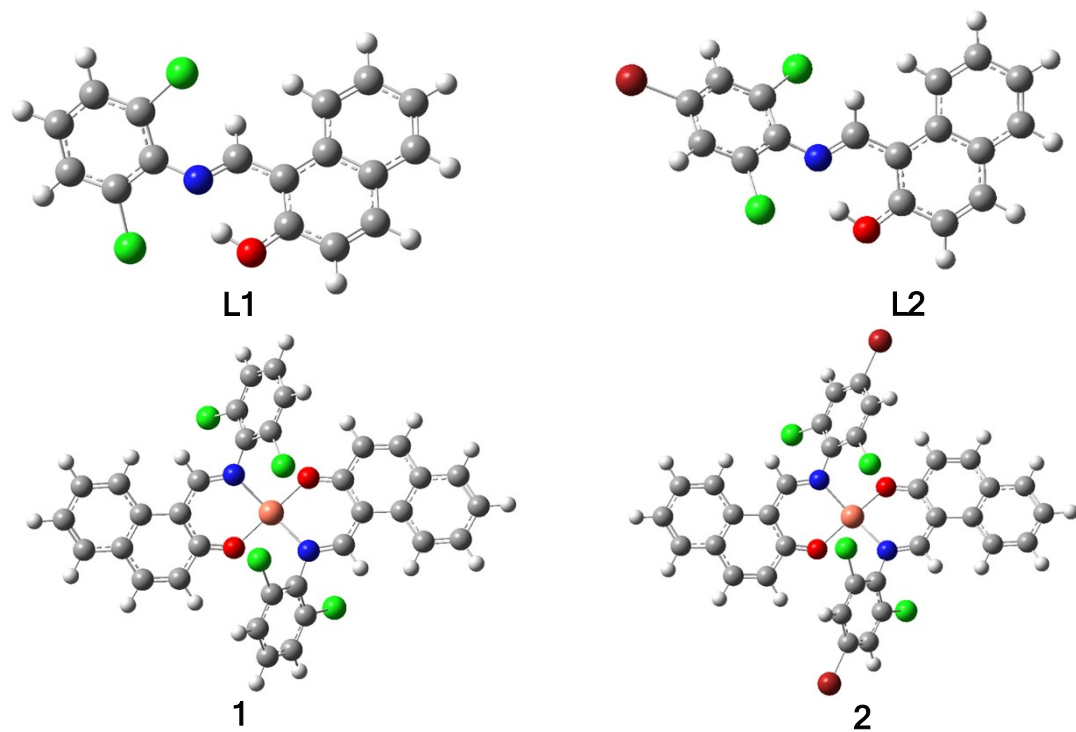


Figure S15: Optimized structures for L1, L2, 1 and 2

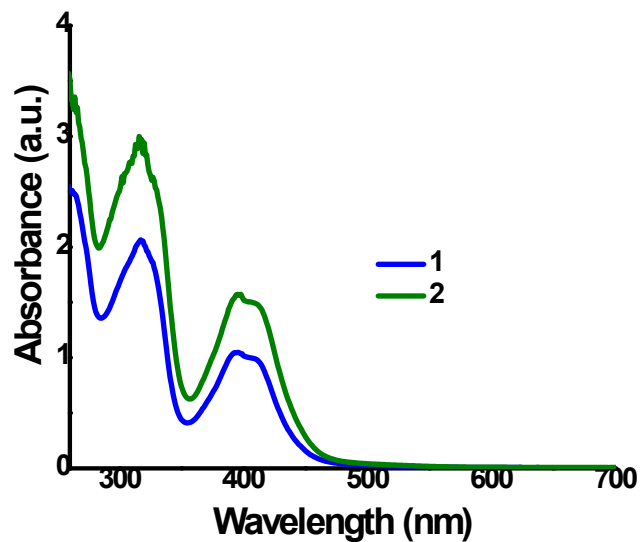


Figure S16(a): Electronic absorption spectra of **1** and **2** at high concentrations

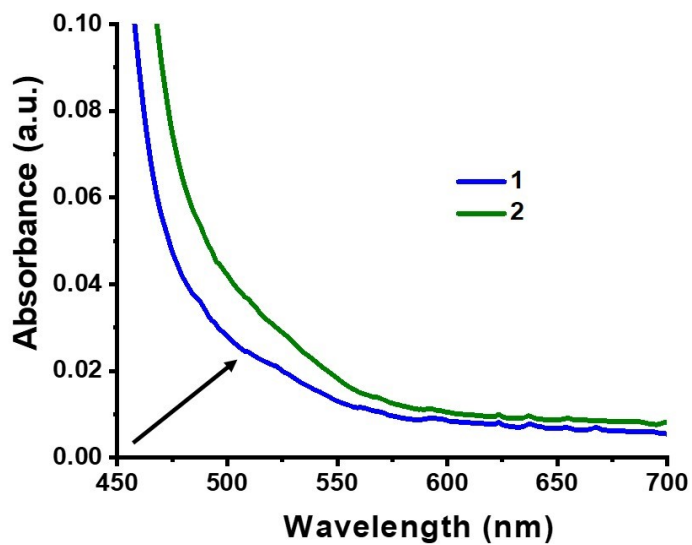


Figure S16(b): Electronic absorption spectra of **1** and **2** at high concentrations showing the weak $d \rightarrow d$ transition.