

Supplementary Data

This supplementary data is a part of a paper entitled “Synthesis, Characterization, Thermal Analysis, DFT, and Computational/Anti-Corrosion Studies for New Azo Metal Complexes”.

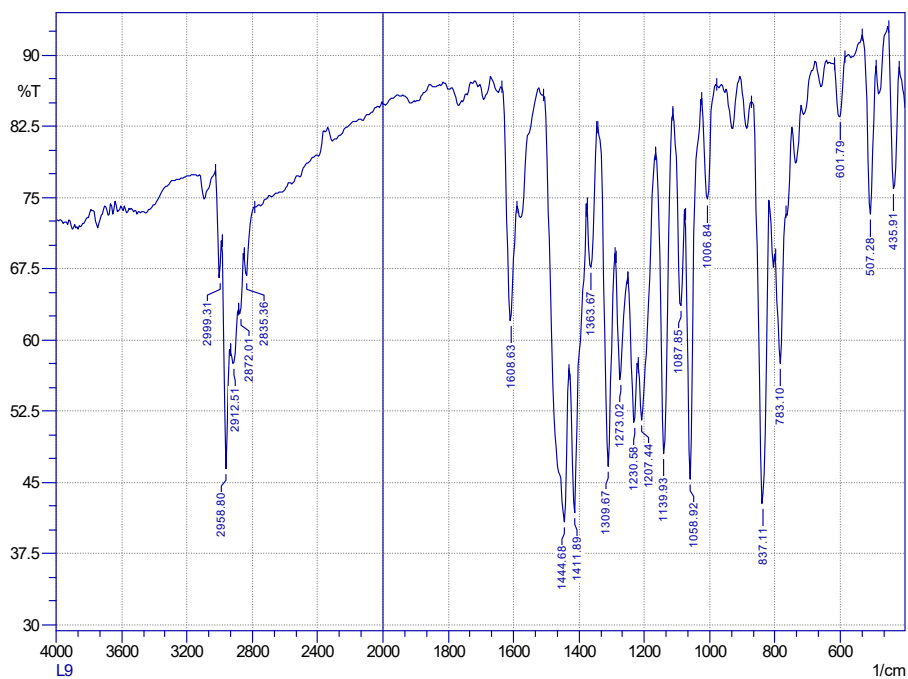


Fig S1. FTIR spectrum of L1

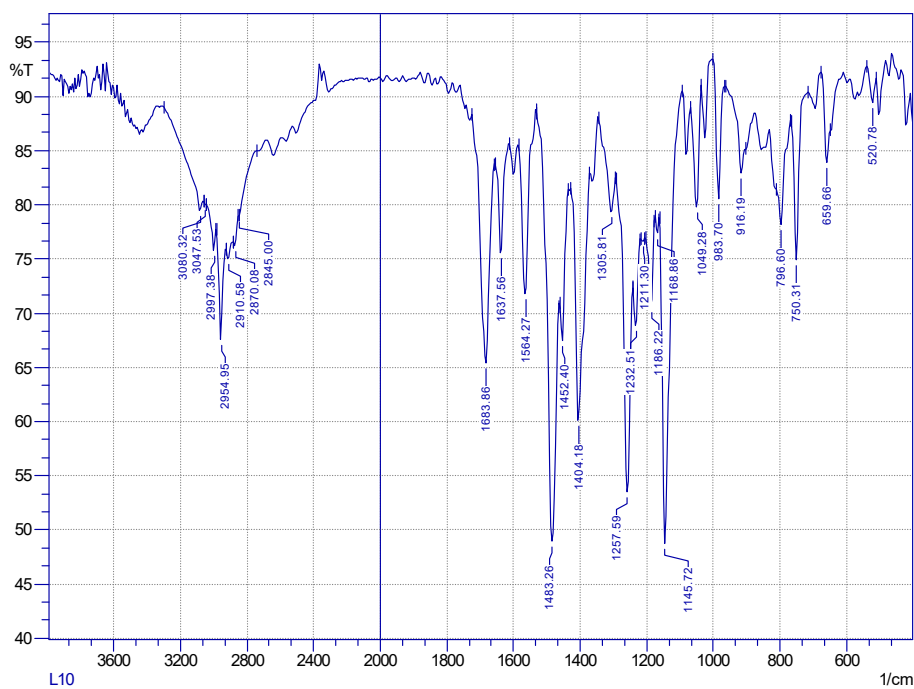
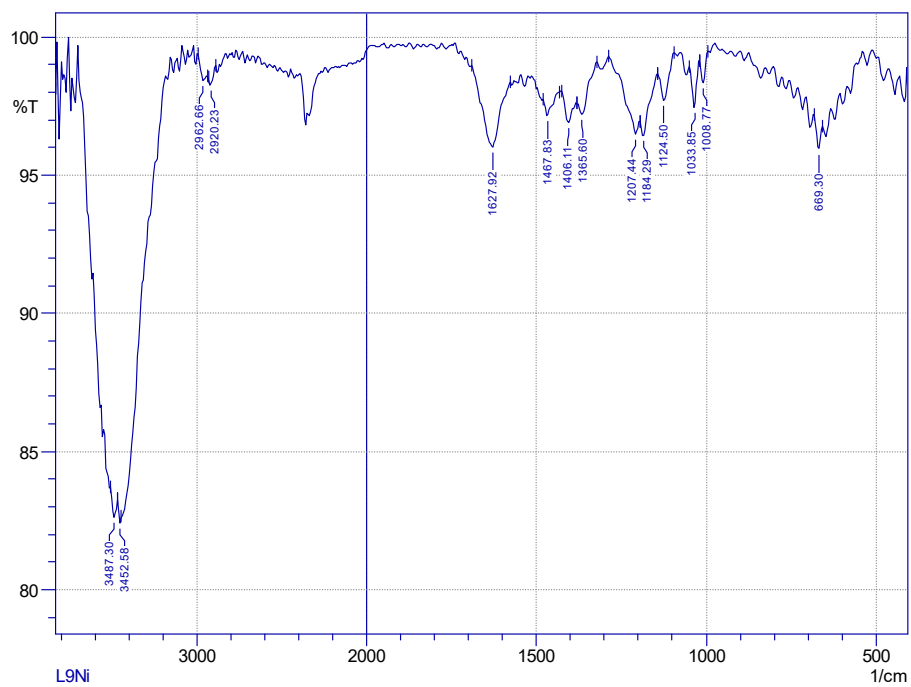
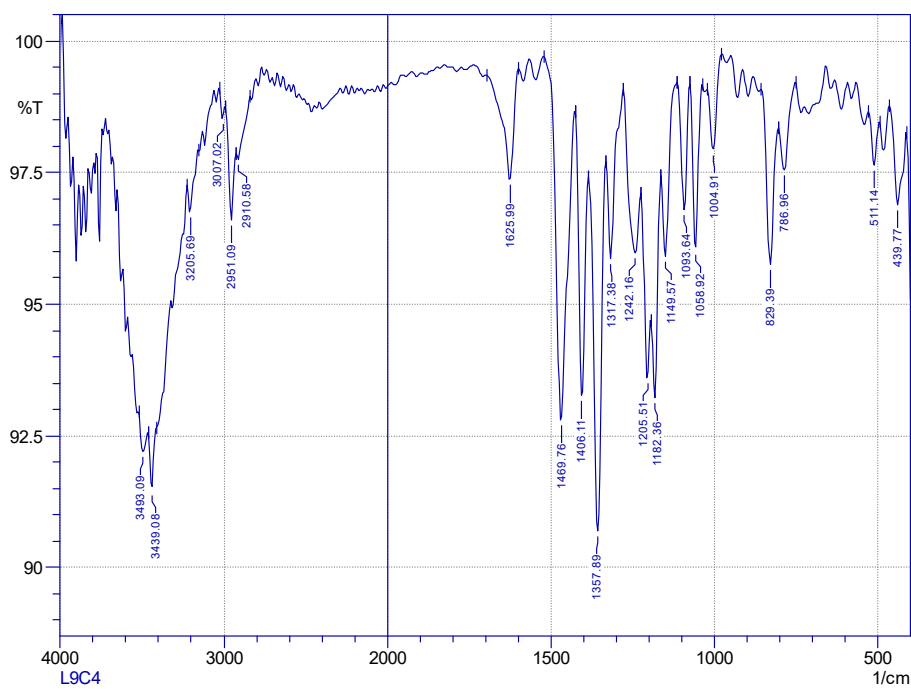
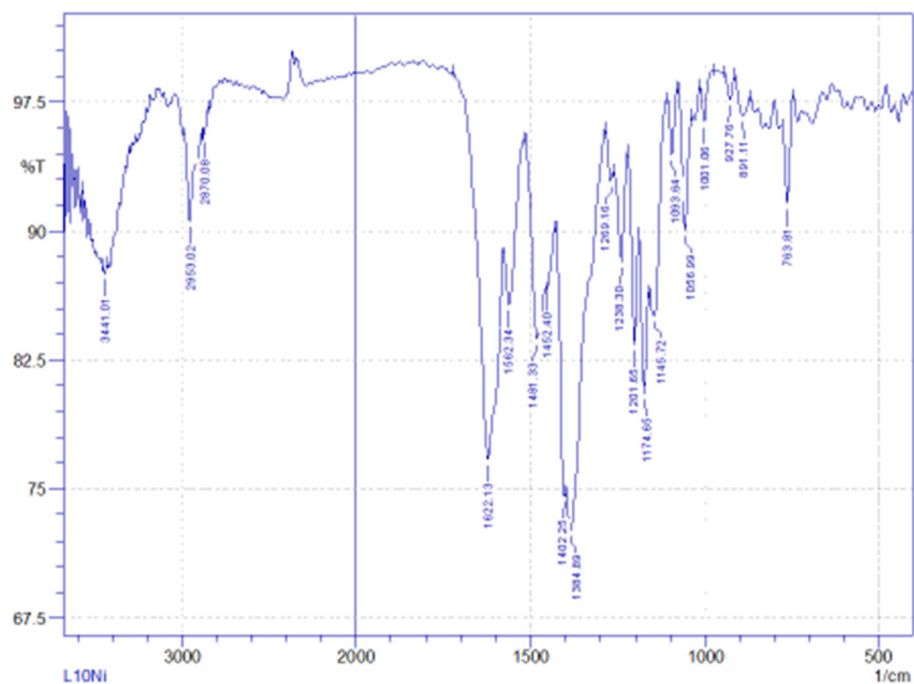
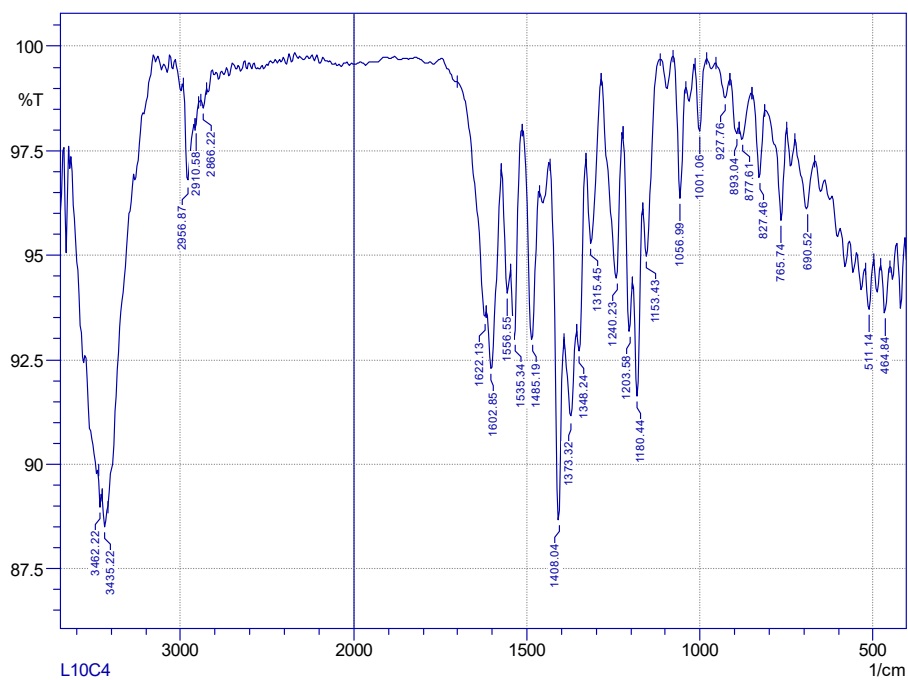
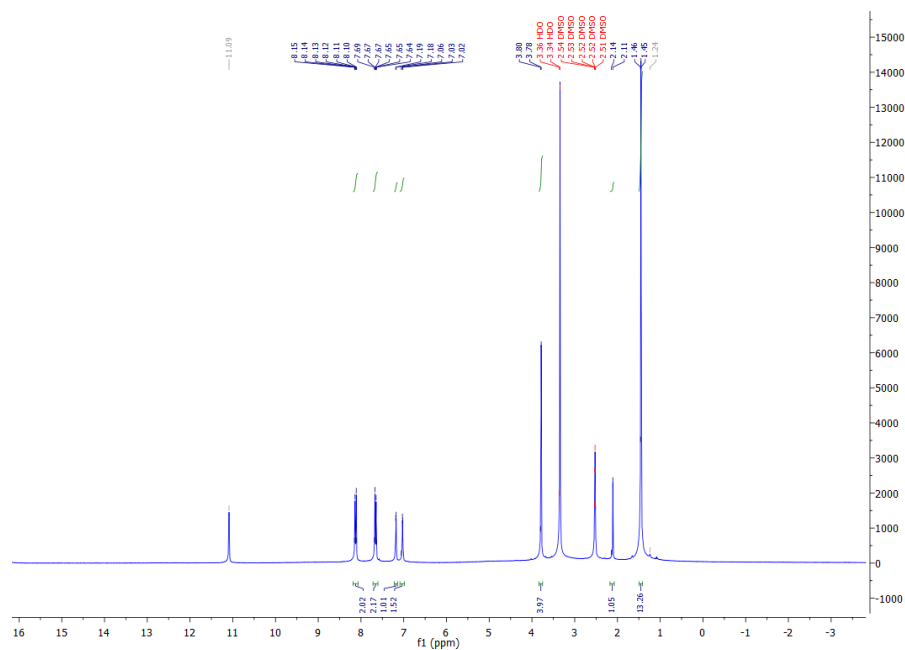
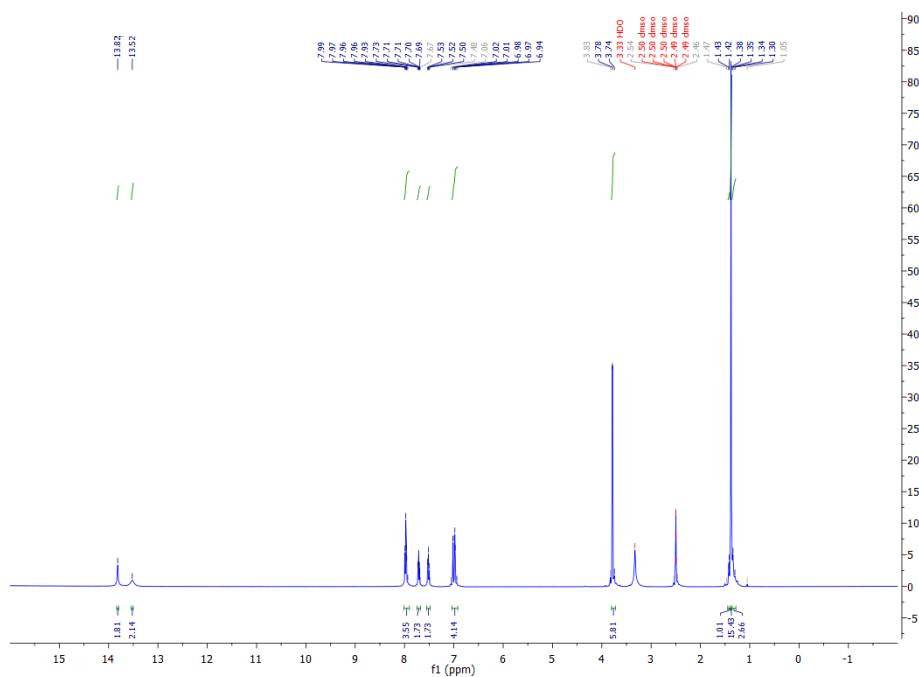
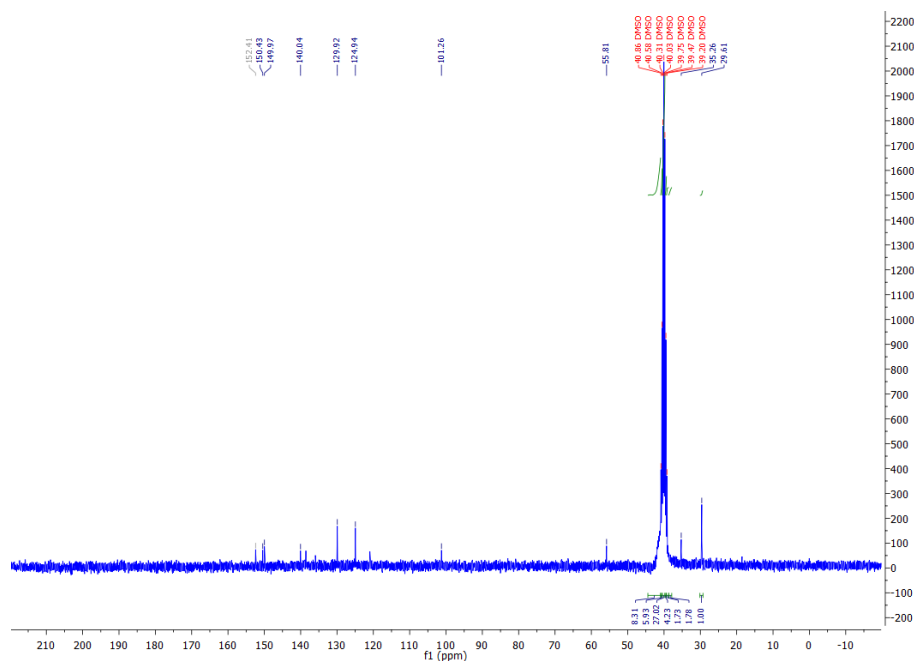
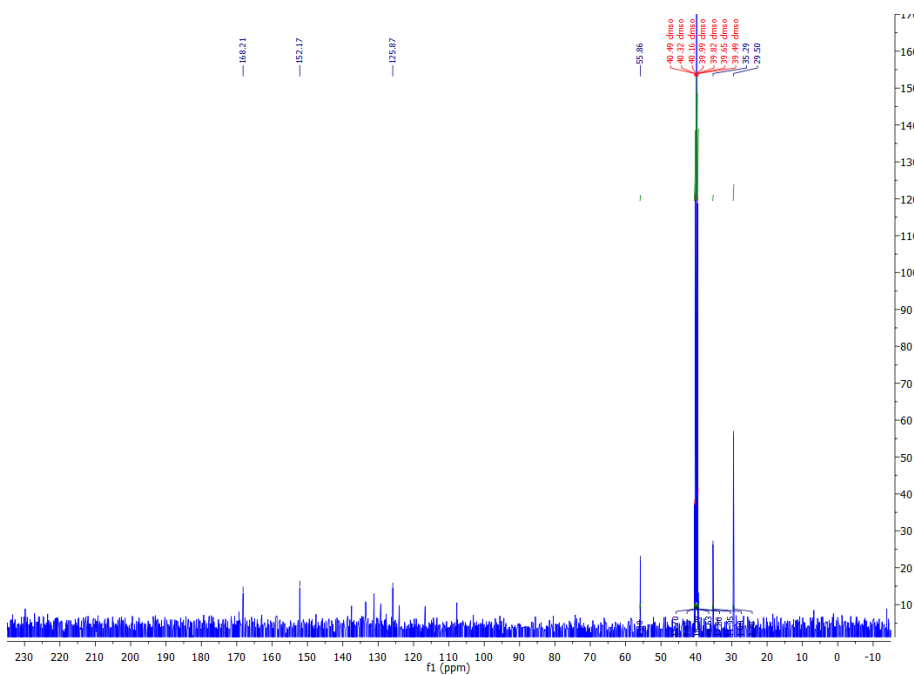


Fig S2. FTIR spectrum of L2

Fig S3. FTIR spectrum of $[\text{NiCl}_2\text{L1}]$ Fig S4. FTIR spectrum of $[\text{CuCl}_2\text{L1}]$

Fig S5. FTIR spectrum of $[\text{NiCl}_2\text{L}_2]$ Fig S6. FTIR spectrum of $[\text{CuCl}_2\text{L}_2]$

Fig S7. ¹H-NMR spectrum of L1Fig S8. ¹H-NMR spectrum of L2

Fig S9. ^{13}C -NMR spectrum of L1Fig S10. ^{13}C -NMR spectrum of L2

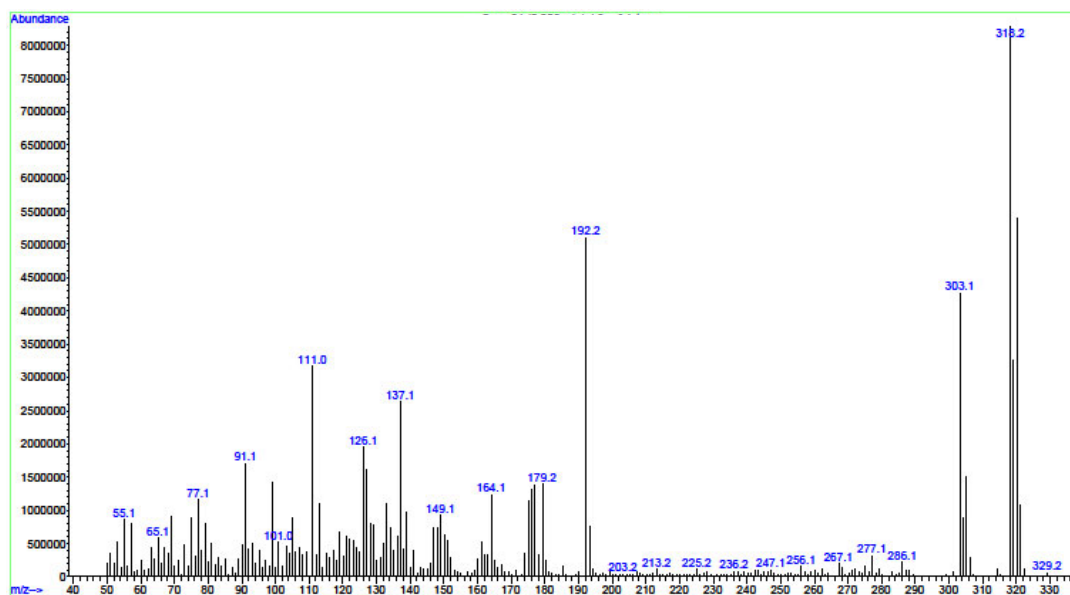


Fig S11. Mass spectrum of L1

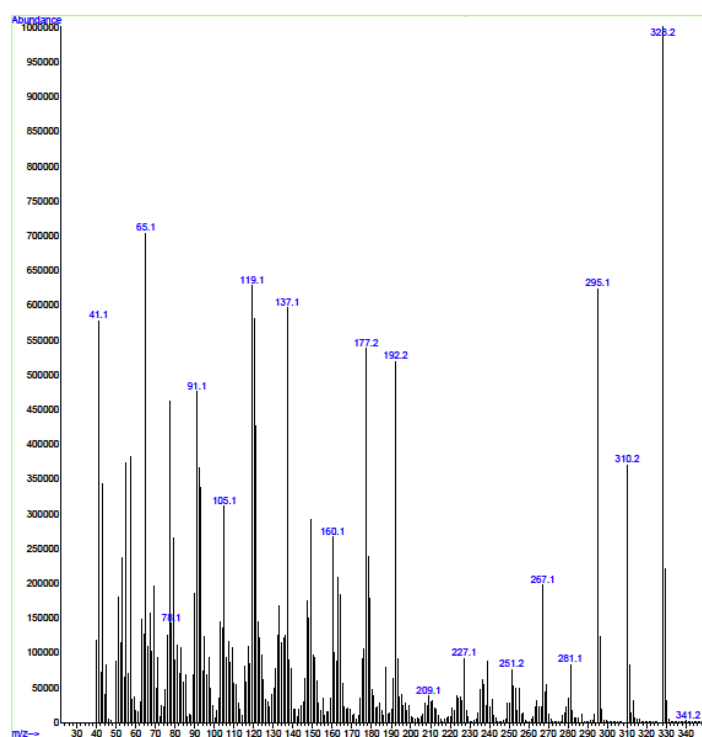
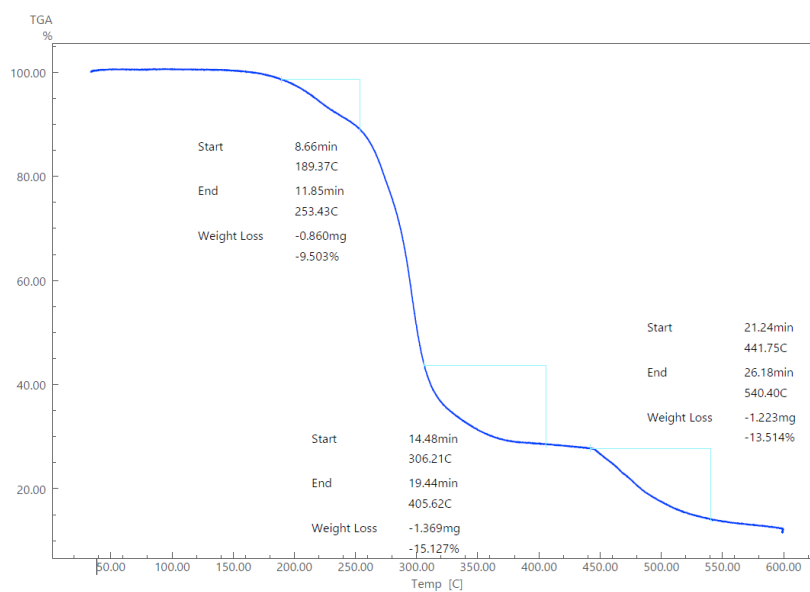
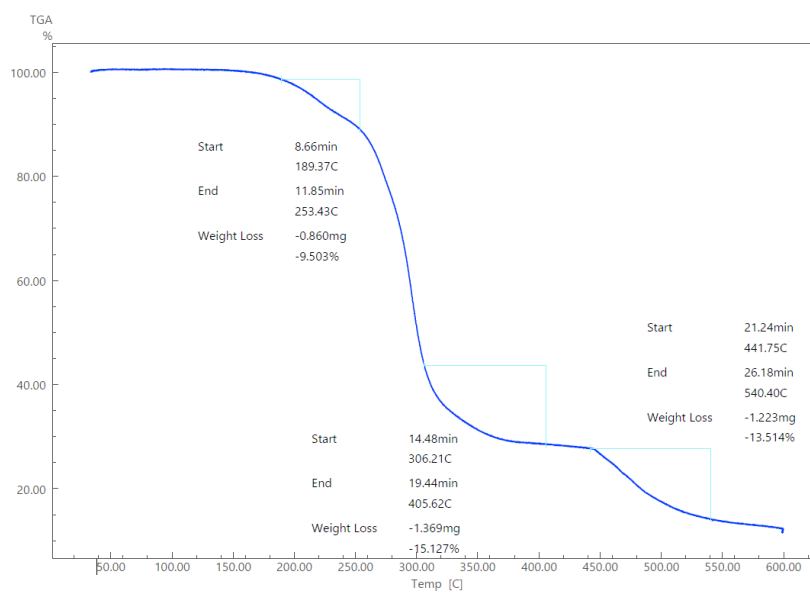


Fig S12. Mass spectrum of L2

Fig S13. TGA plot of $[\text{NiCl}_2\text{L1}]$ Fig S14. TGA plot of $[\text{CuCl}_2\text{L1}]$

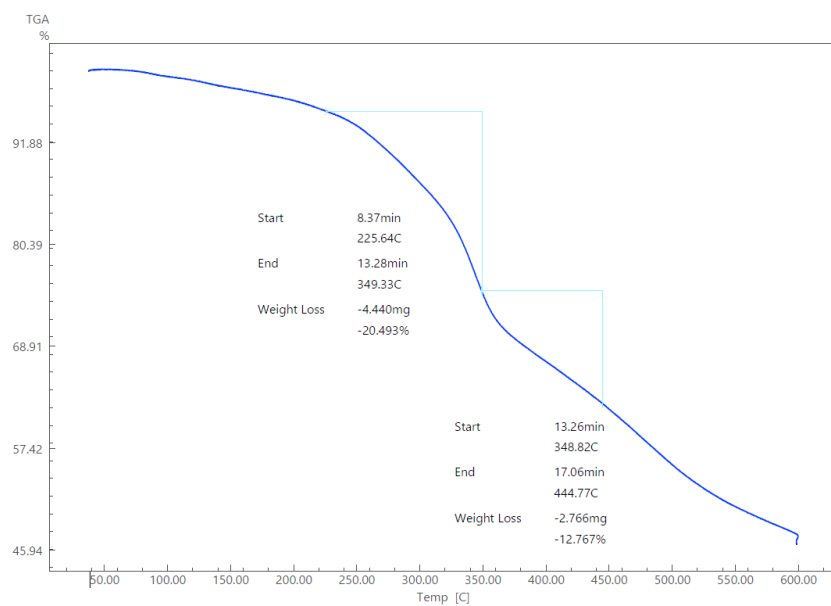
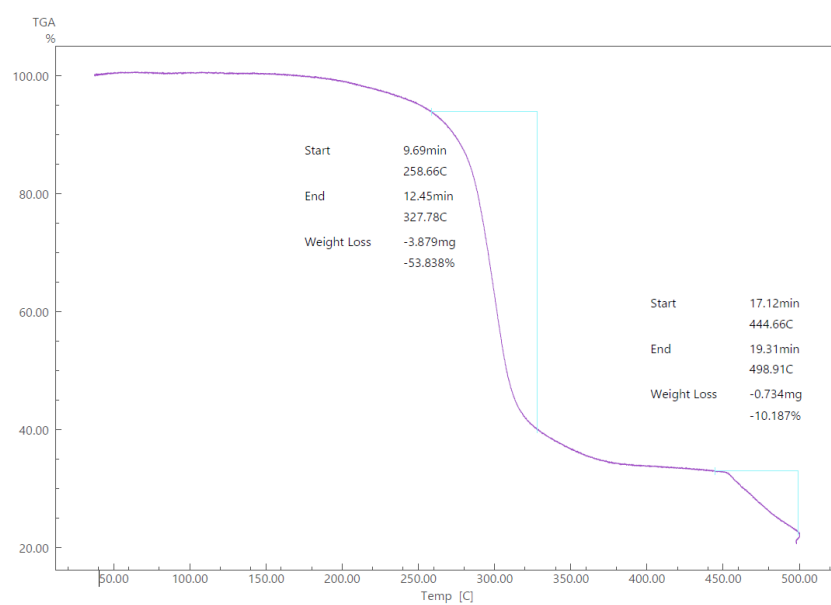
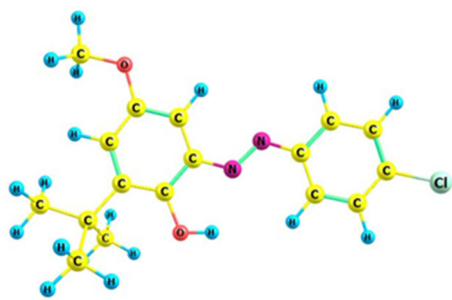
Fig S15. TGA plots of $[\text{NiCl}_2\text{L}_2]$ Fig S16. TGA plots of $[\text{CuCl}_2\text{L}_2]$ 

Fig S17. Optimized structure of L1

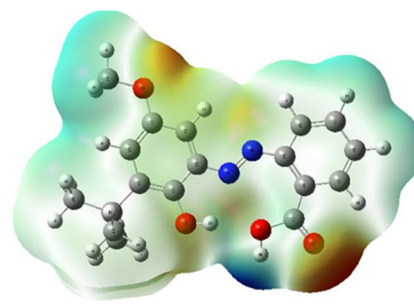


Fig S18. Electronic surface potential of L2

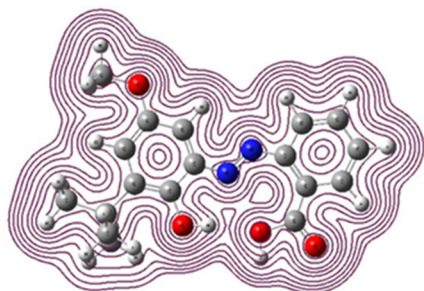


Fig S19. Electrostatic potential map of L2

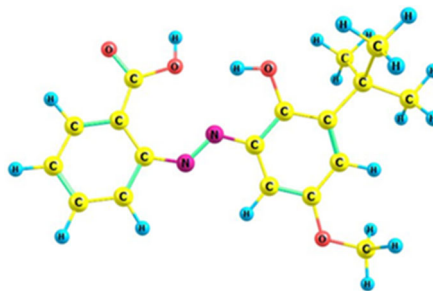


Fig S20. Optimized structure of L2

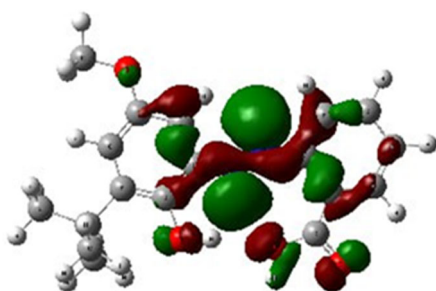


Fig S21. HOMO of L2

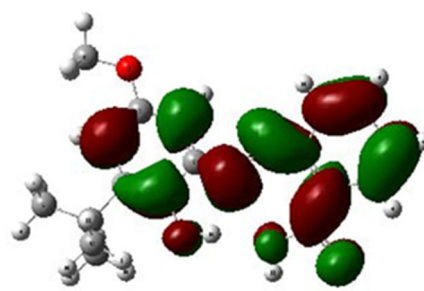


Fig S22. LUMO of L2

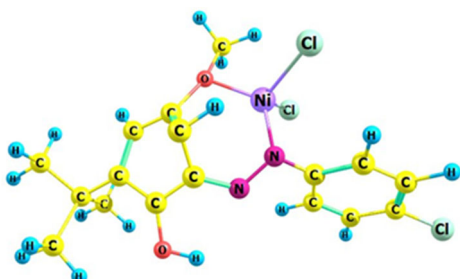


Fig S23. Optimized structure of $[\text{NiCl}_2\text{L1}]$

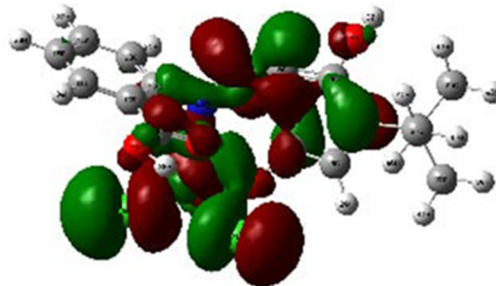


Fig S24. HOMO of $[\text{NiCl}_2\text{L1}]$

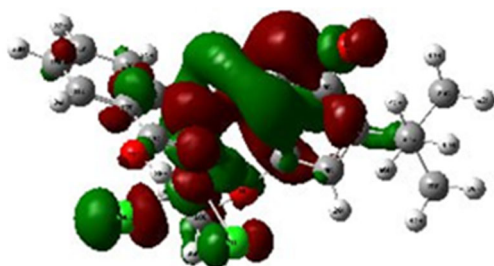


Fig S25. LUMO of $[\text{NiCl}_2\text{L1}]$

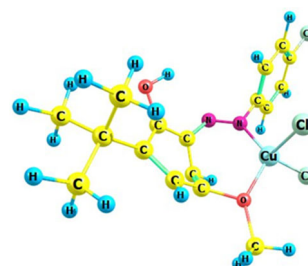
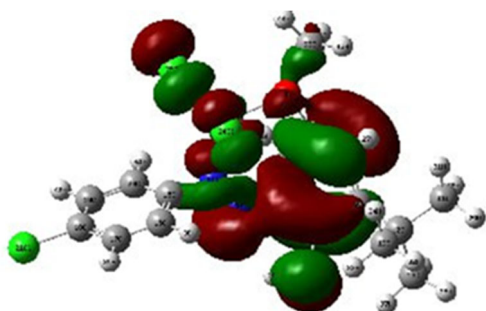
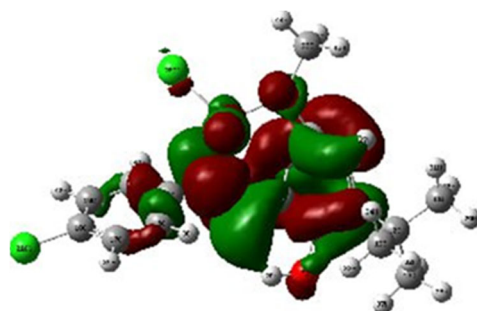
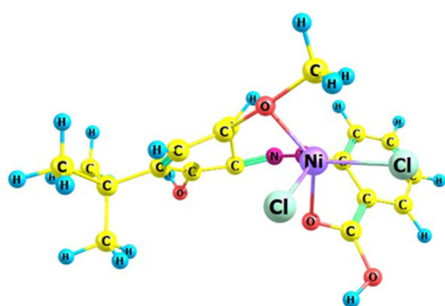
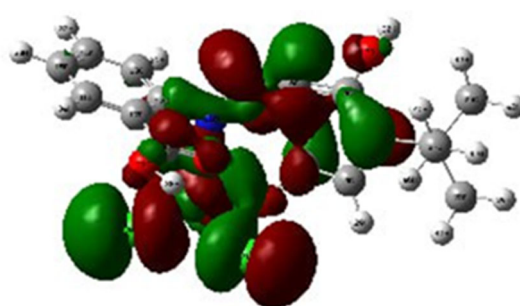
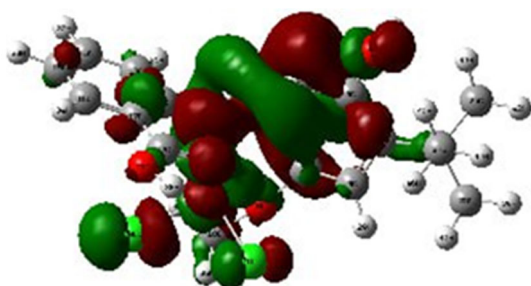
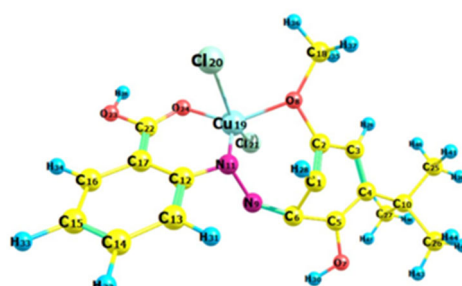
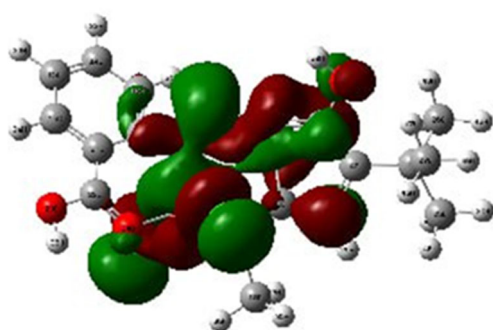
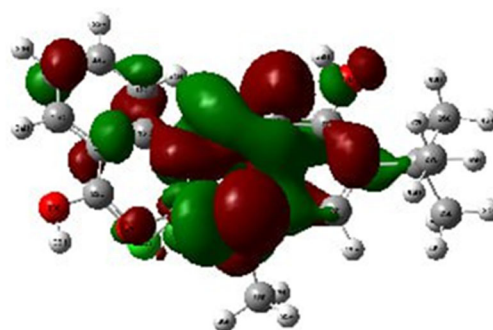


Fig S26. Optimized structure of $[\text{CuCl}_2\text{L1}]$

Fig S27. HOMO of $[\text{CuCl}_2\text{L1}]$ Fig S28. LUMO of $[\text{CuCl}_2\text{L1}]$ Fig S29. Optimized structure of $[\text{NiCl}_2\text{L2}]$ Fig S30. HOMO of $[\text{NiCl}_2\text{L2}]$ Fig S31. LUMO of $[\text{NiCl}_2\text{L2}]$ Fig S32. Optimized structure of $[\text{CuCl}_2\text{L2}]$ Fig S33. HOMO of $[\text{CuCl}_2\text{L2}]$ Fig S34. LUMO of $[\text{CuCl}_2\text{L2}]$