Supplementary Information (SI) for RSC Advances.
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Spectroscopic, computational, and biological activity studies of bivalent metal complexes of (*E*)-N'-(4-(dimethylamino)benzylidene) isonicotinohydrazide

Osama'a A. Y.Al-Samrai[1], Mohamed E Eissa[2], Khalid Tuama Abdullah [3], Tarek A. Yousef [2*], Mona H Alhalafi[4], Ahmed S. M. Al-Janabi [5*],

[1] *Department of Chemistry, College of Education for Pure Sciences, University of Samarra, Samarra, Iraq*

[2]*College of Science, Chemistry Department, Imam Mohammad Ibn Saud Islamic University (IMSIU), Riyadh 11623, Saudi Arabia*

[3]*Department of Chemistry, College of Education for Pure Science, University of Diyala, Diyala, Iraq*

[4]*Department of Chemistry, College of Science Al-Zulfi, Majmaah University, Al-Majmaah 11952, Saudi Arabia*

[5] *Department of Chemistry, College of Science, Tikrit University, Tikrit, Iraq*

Fig. SI 1. Theoretical and Experimental FT-IR spectra of the **HL** Ligand calculated at the B3LYP/6-31G+(d,p) level with frequency scaling using CCCBDB factors **0.964**.

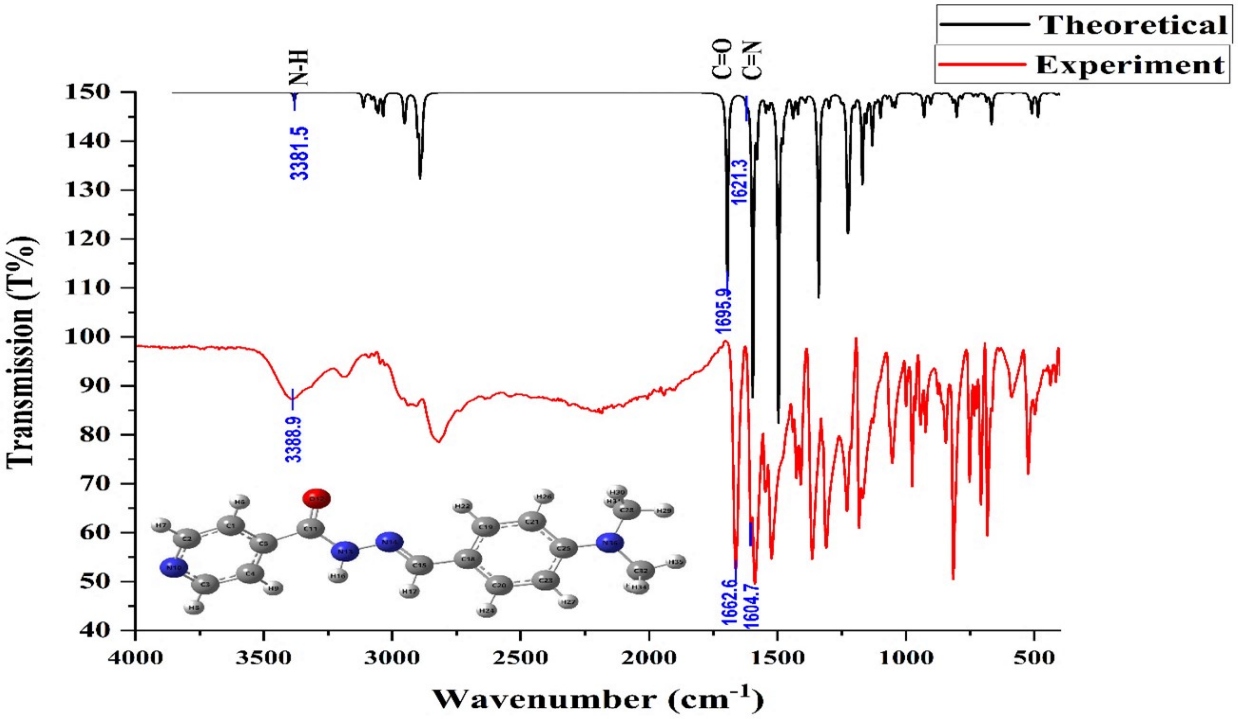


Fig. SI 2. Theoretical and Experimental FT-IR spectra of the **complex (1)** calculated at the B3LYP/6-31G+(d,p) level with frequency scaling using CCCBDB factors **0.964**.

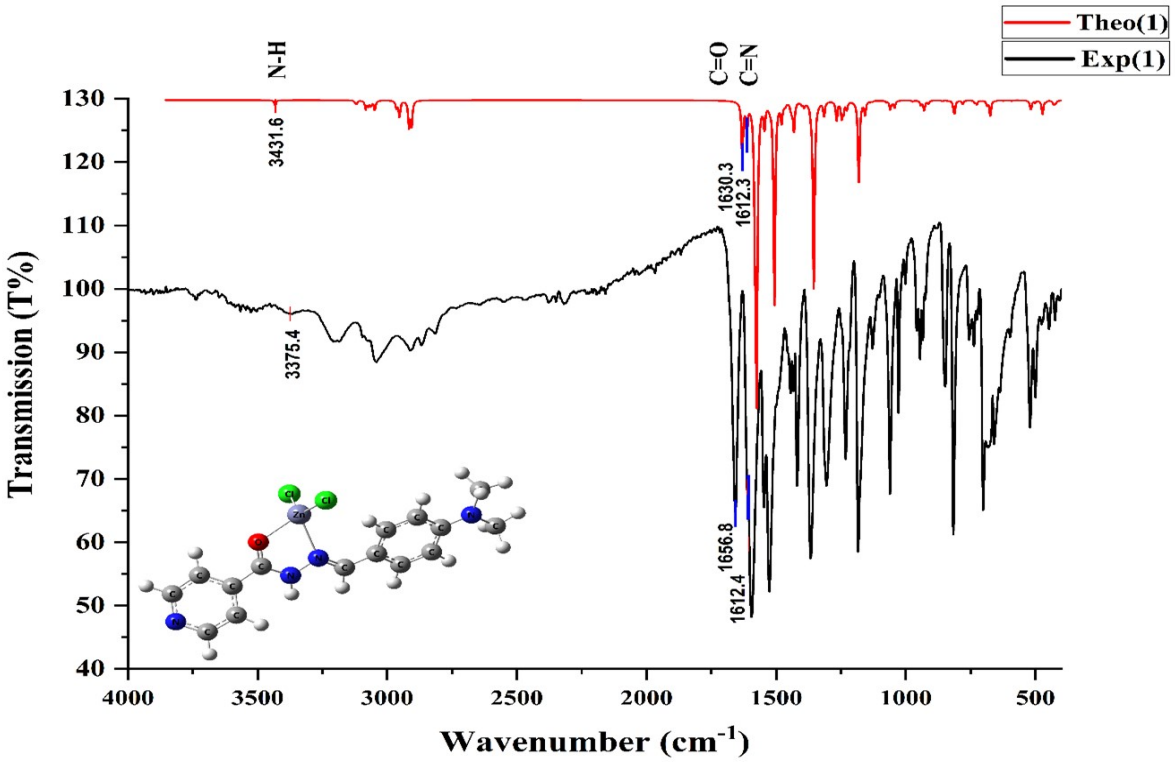


Fig. SI 3. Theoretical and Experimental FT-IR spectra of the **complex (3)** calculated at the B3LYP/6-31G+(d,p) level with frequency scaling using CCCBDB factors **0.964**.

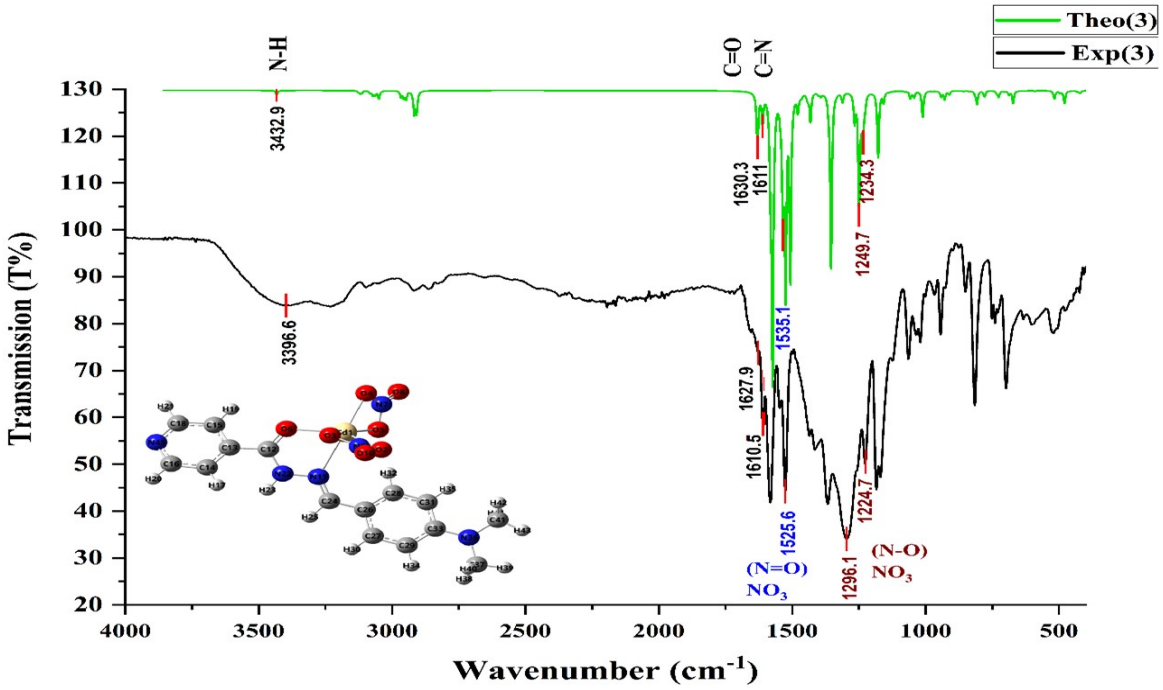


Fig. SI 4. Theoretical and Experimental FT-IR spectra of the **complex (4)** calculated at the B3LYP/6-31G+(d,p) level with frequency scaling using CCCBDB factors **0.964**.

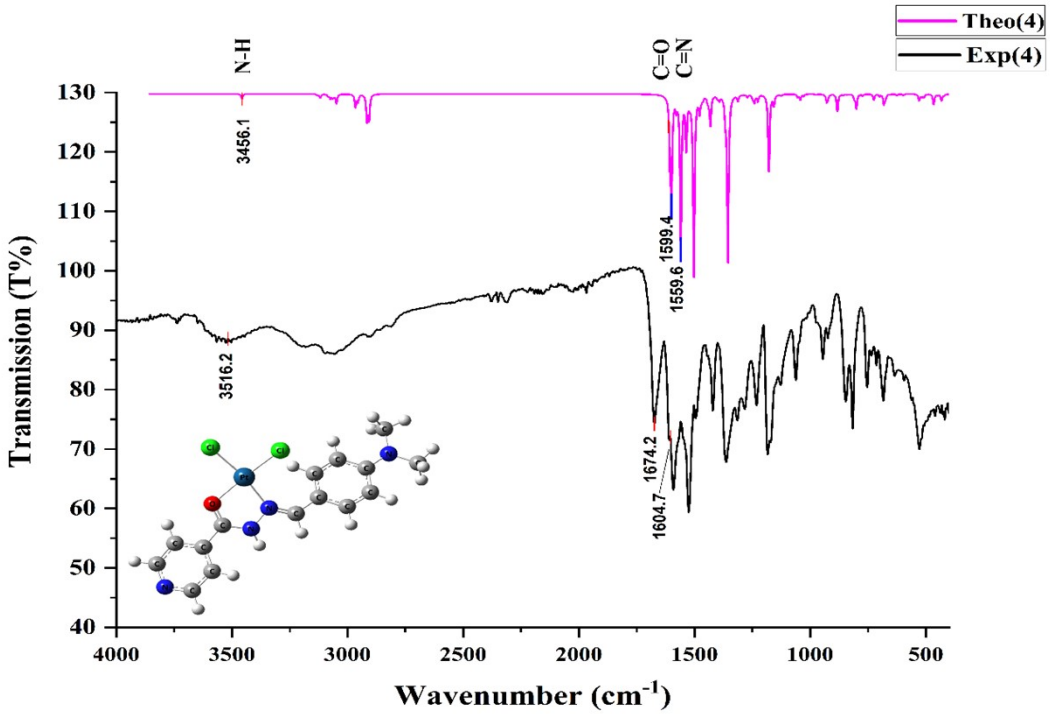


Fig. SI 5. ^{1}H NMR spectrum of the **HL** Ligand

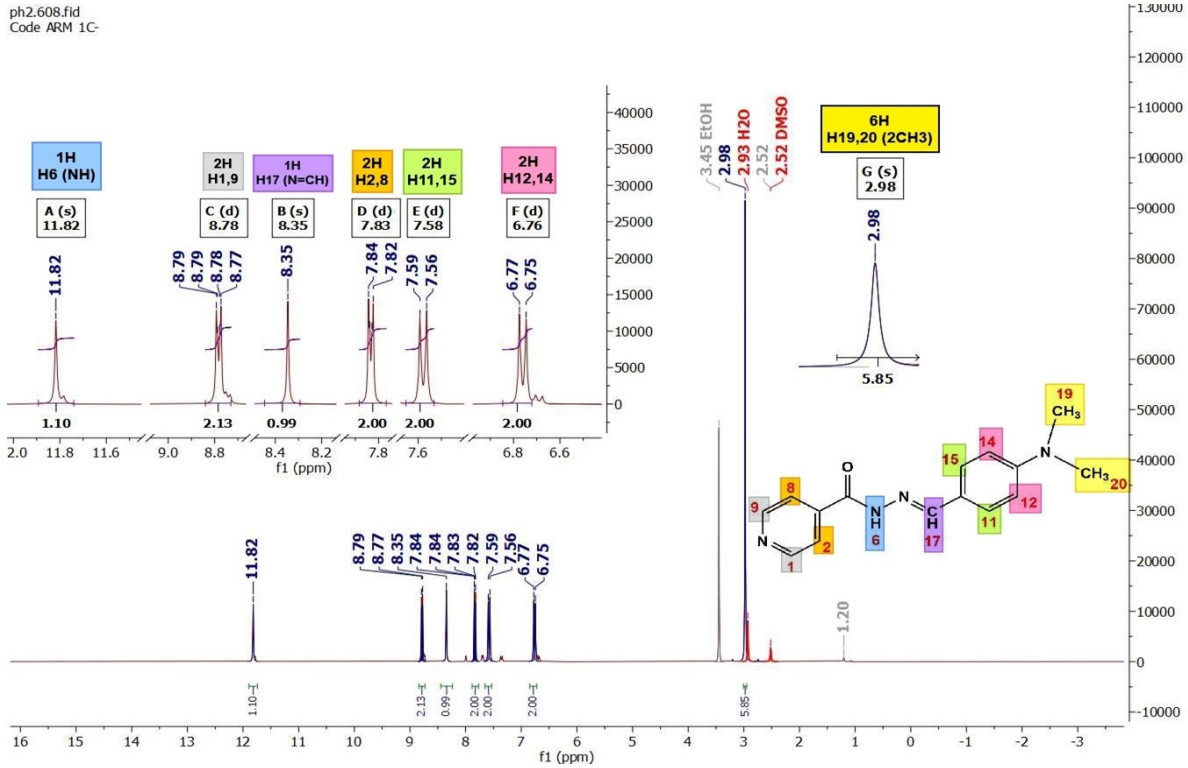


Fig. SI 6. ^{1}H NMR spectrum of the **complex (1)**

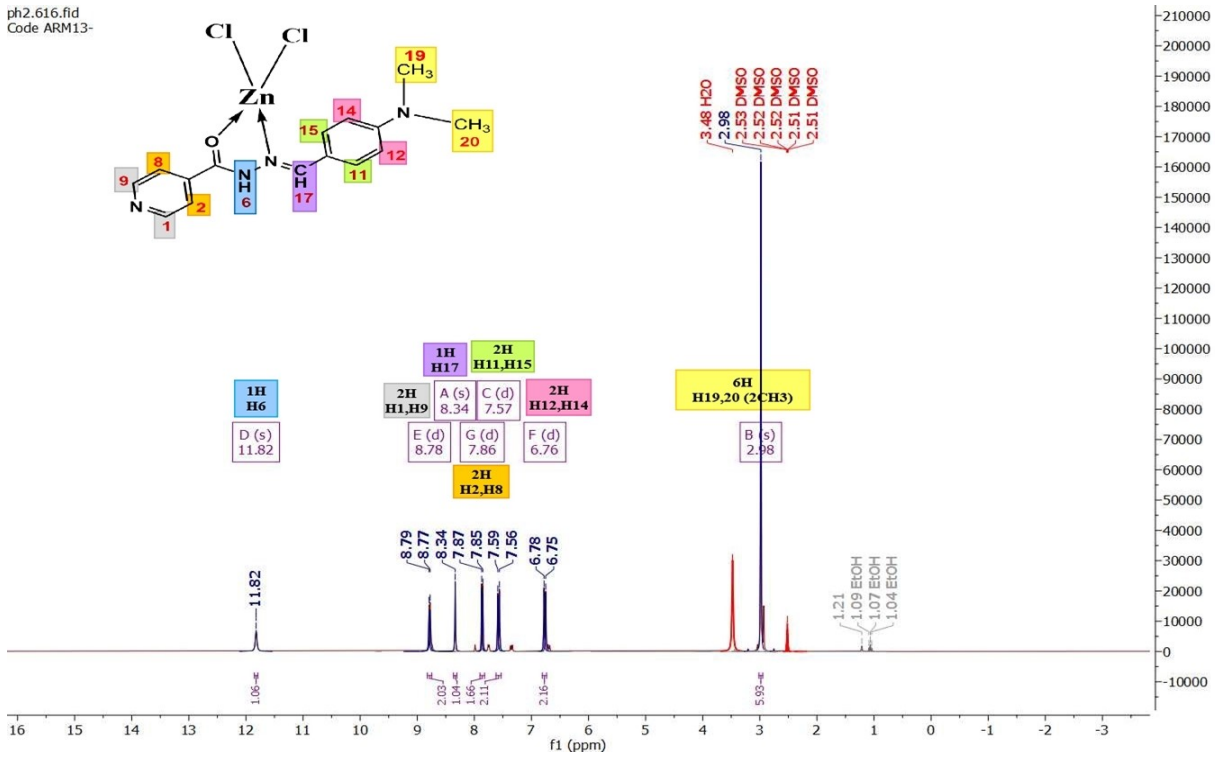


Fig. SI 7. ^{1}H NMR spectrum of the **complex (2)**

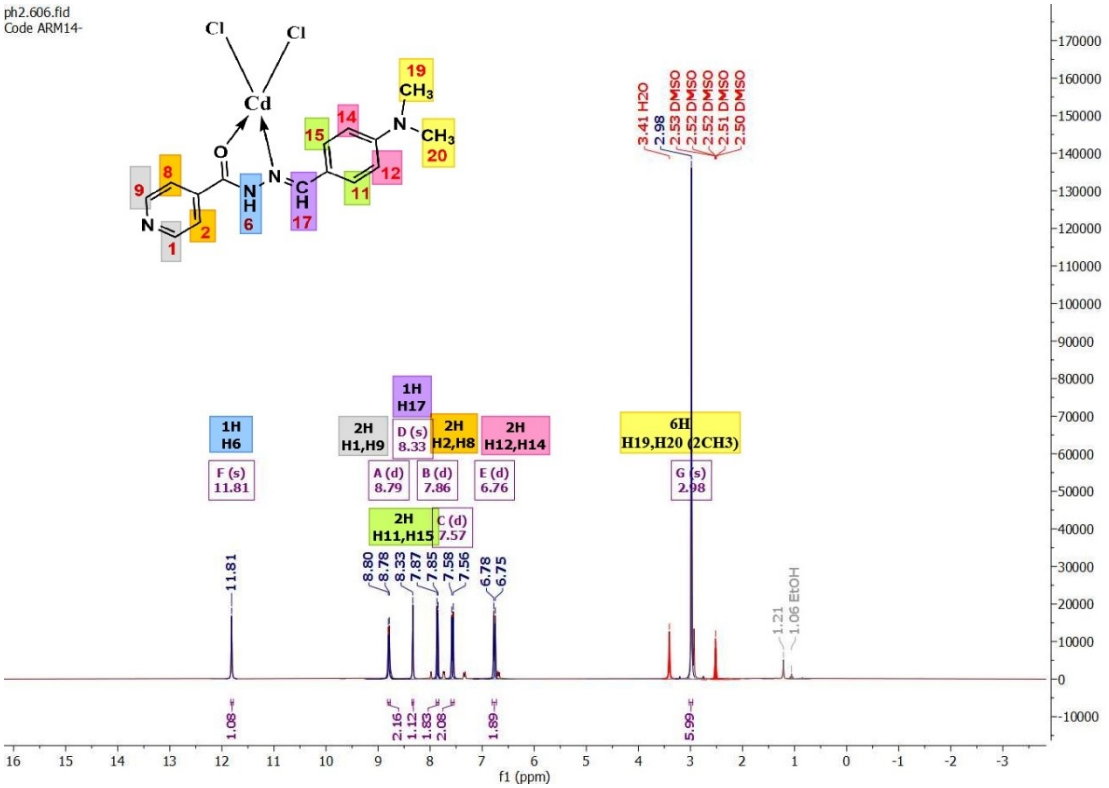


Fig. SI 8. ^{1}H NMR spectrum of the **complex (3)**

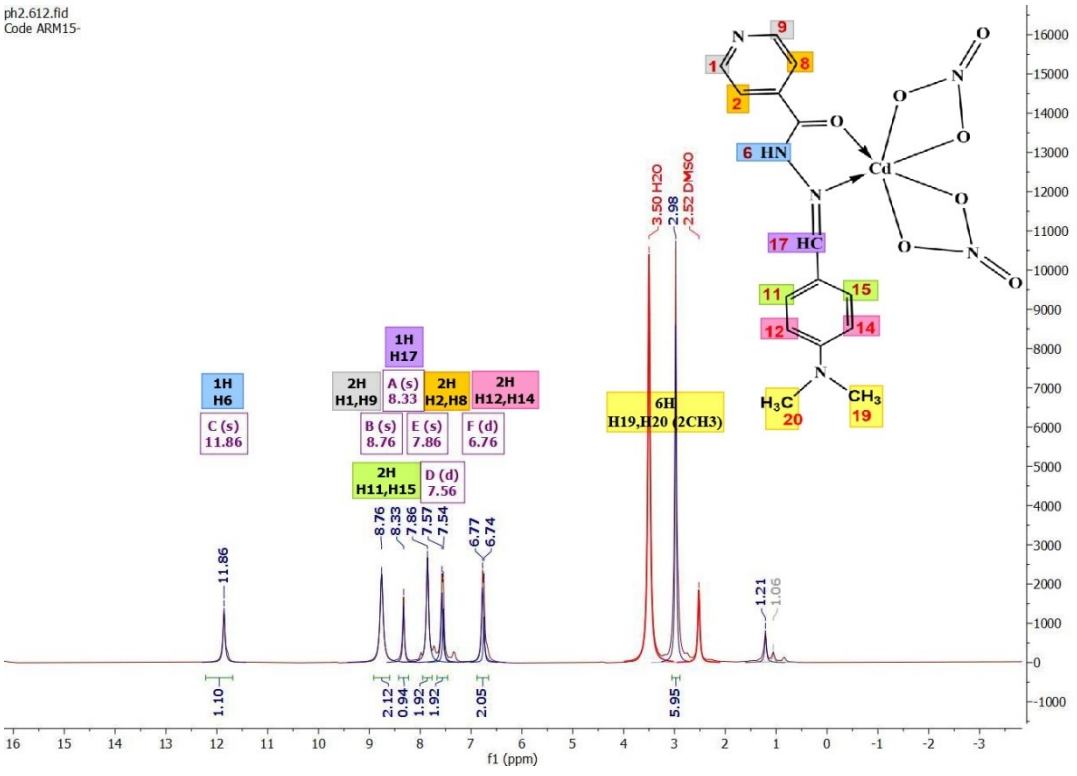


Fig. SI 9. ^{1}H NMR spectrum of the **complex (4)**

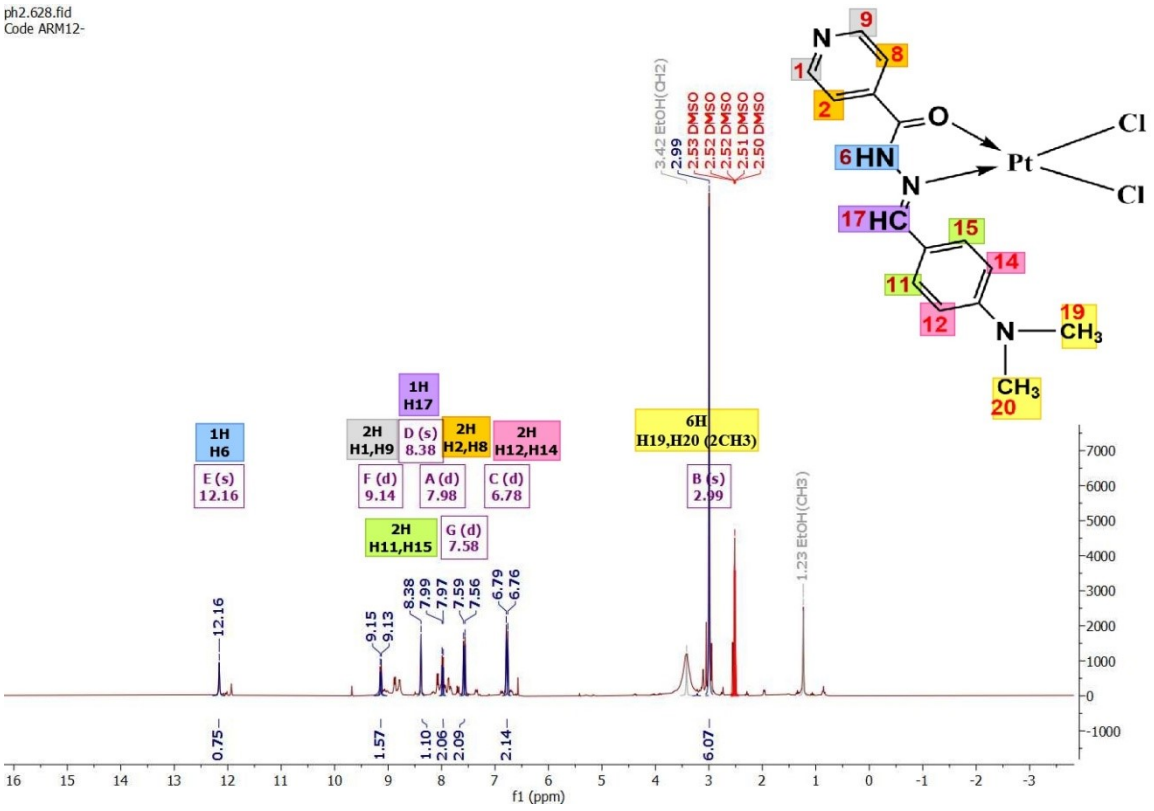


Fig. SI 10. ^{13}C NMR spectrum of the **HL** Ligand

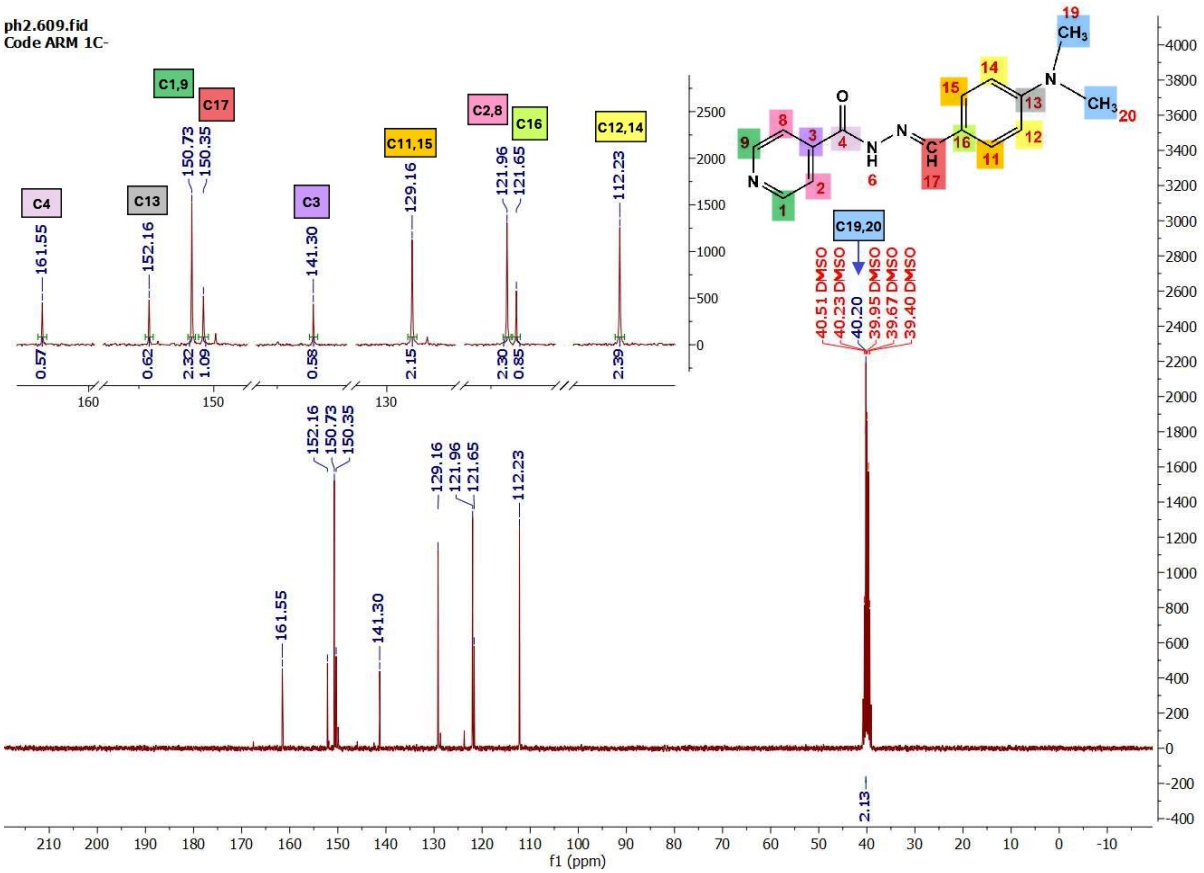


Fig. SI 11. ^{13}C NMR spectrum of the **complex (1)**

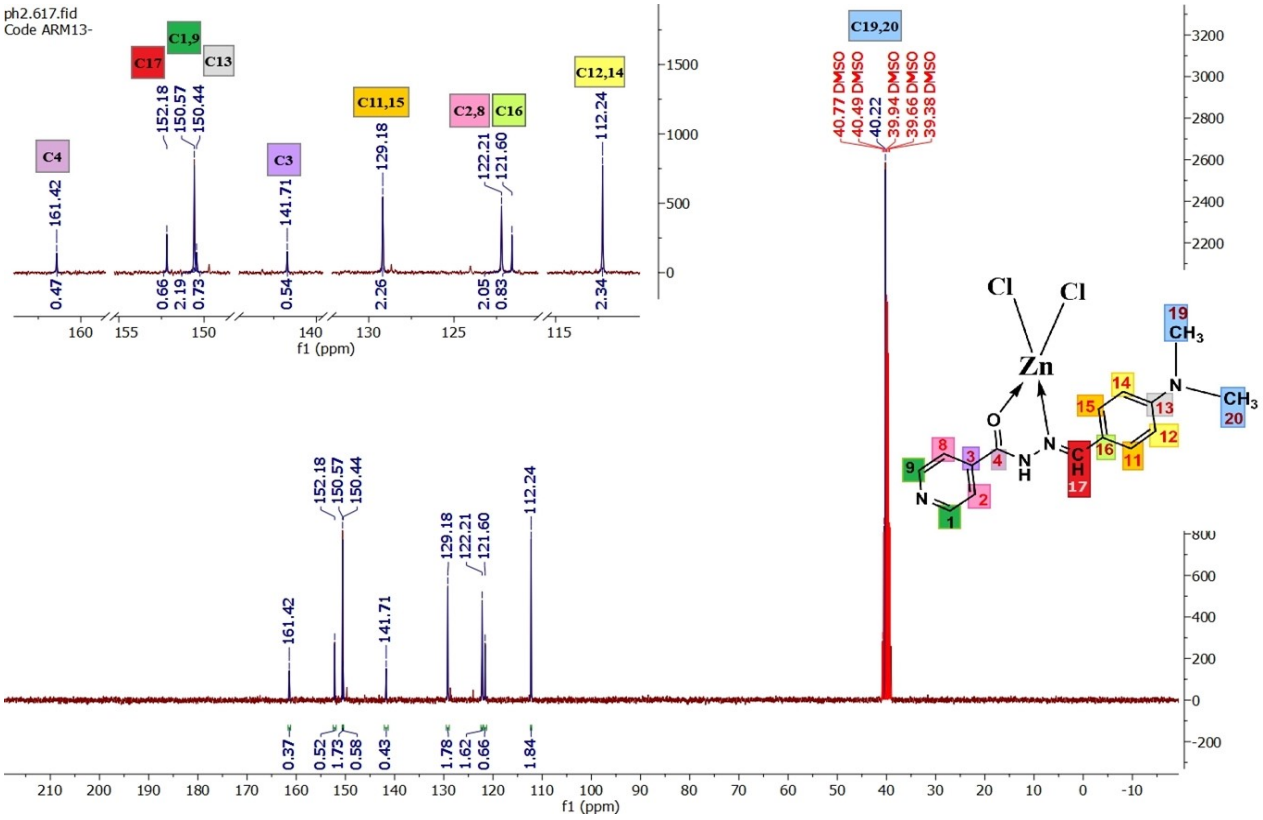


Fig. SI 12. ^{13}C NMR spectrum of the **complex (2)**

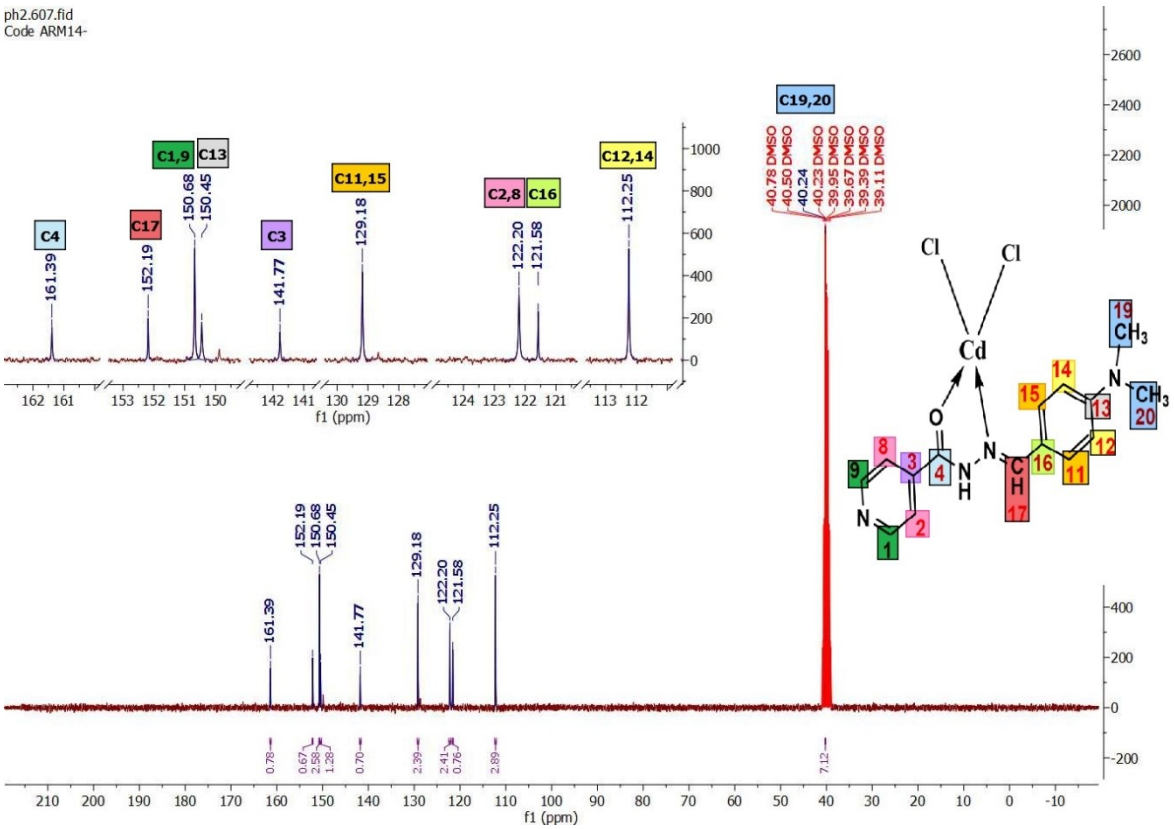


Fig. SI 13. ^{13}C NMR spectrum of the **complex (3)**

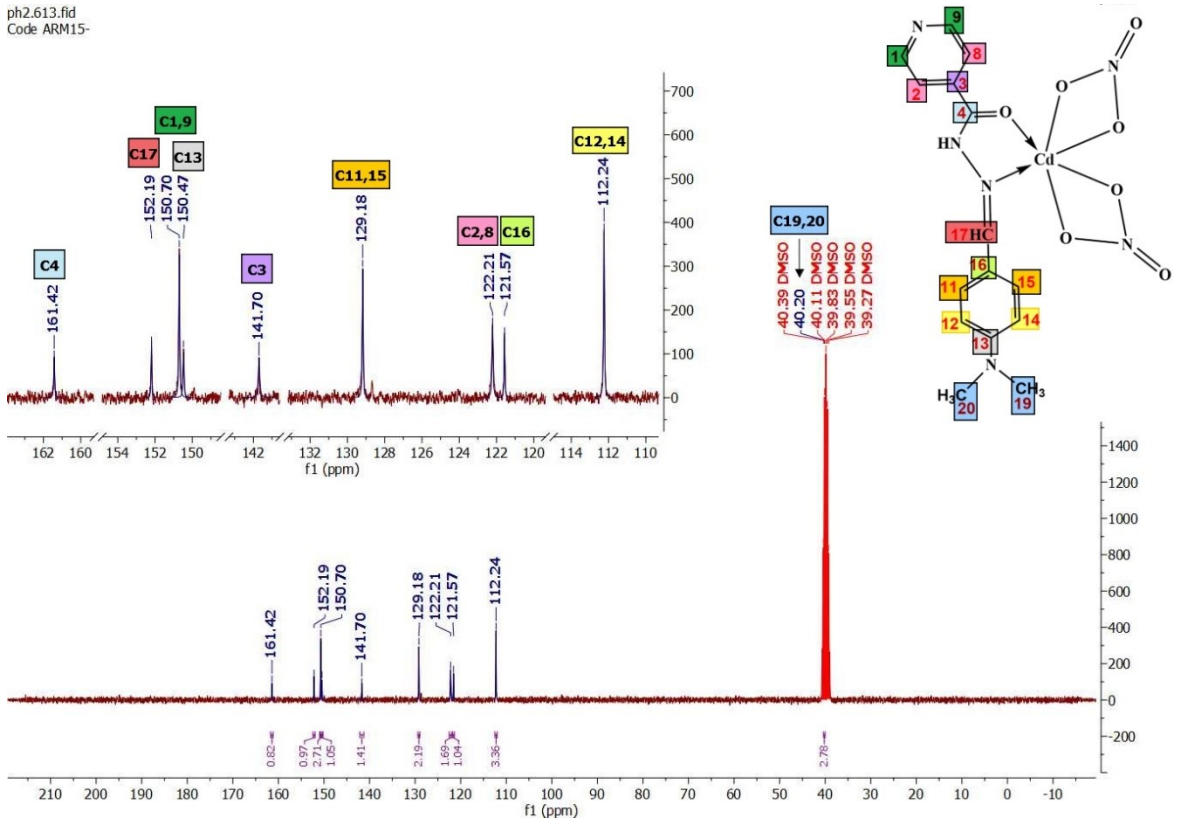
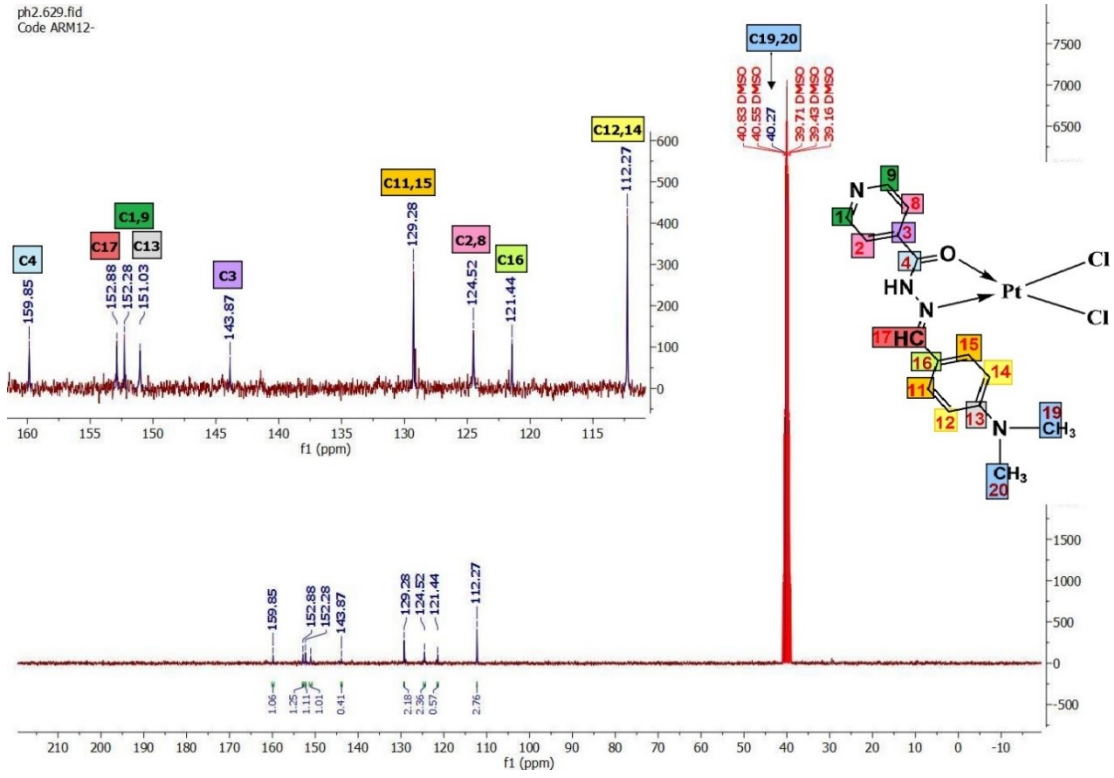


Fig. SI 14. ^{13}C NMR spectrum of the **complex (4)**



Exp. SI 1 Anti-bacterial activity

Two pathogenic bacterial species (*Escherichia coli* and *Staphylococcus aureus*) were utilized to assess the antimicrobial activity of the synthesized complexes and free ligands. The antibacterial activity of the synthesized complexes was evaluated at concentrations of 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}, and 10^{-6} M of solutions, and the effects were compared to the streptomycin drug, and DMSO is a negative control. The agar disc diffusion method, as initially proposed by Bauer, was employed to evaluate the antibacterial characteristics of the complexes [Bauer, A. W., PERRY, D. M., & KIRBY, W. M. (1959). Single-disk antibiotic-sensitivity testing of staphylococci: An analysis of technique and results. *AMA archives of internal medicine*, *104*(2), 208-216.]. All plates seeded at 37 °C were incubated for 24 hours, and the well was determined in the DIZ.