**Heteroatom Chemistry**

**Computational Studies of 4-formylpyridinethiosemicarbazone, Structural and Biological studies of its Ni(II)and Cu(II)complexes**

Mydhili P. Sripathi, 1 Sireesha Berely, 1 Venkata Ramana Reddy Chittireddy2

1 Department of Chemistry, Nizam College, Osmania University, Hyderabad, India

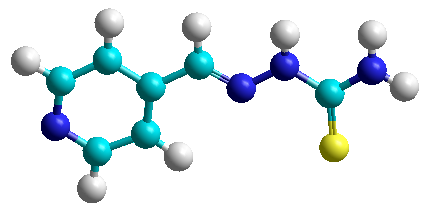
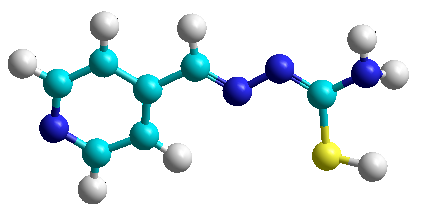
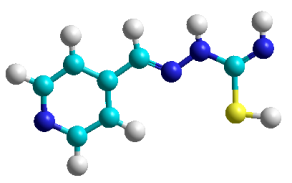
2 Department of Chemistry, Jawaharlal Nehru Technological University Hyderabad, Hyderabad, India

E-mail: vrr9@jntuh.ac.in

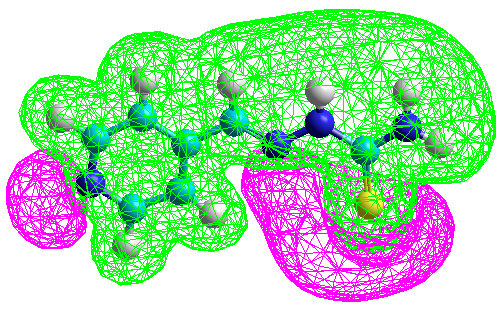
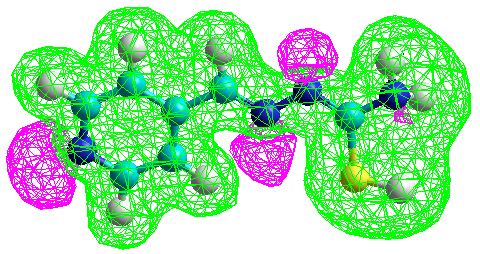
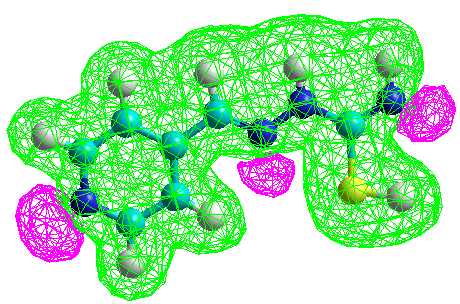
**Supplementary Material**

Figures

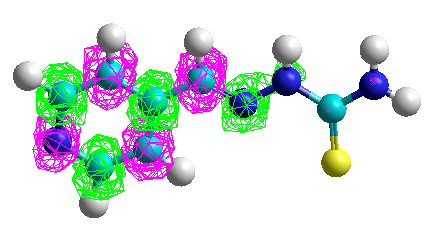
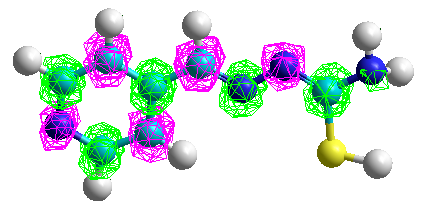
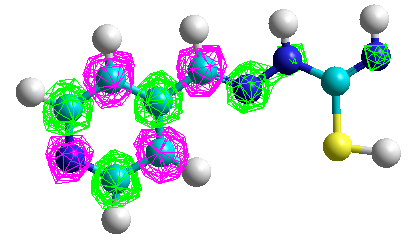
Thione Thiol-1 Thiol-2

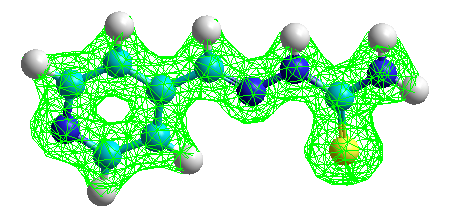
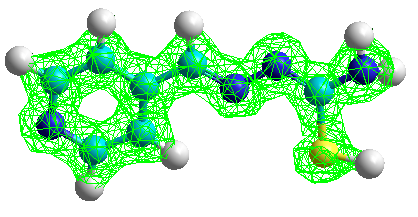
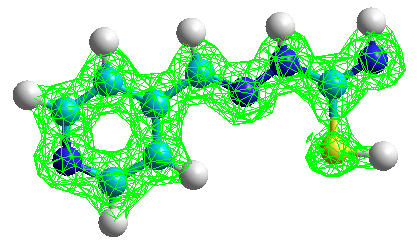
Optimized Geometry

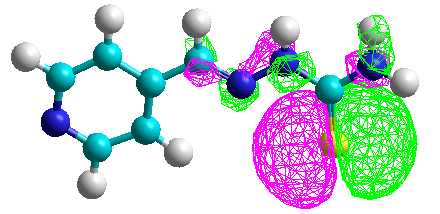
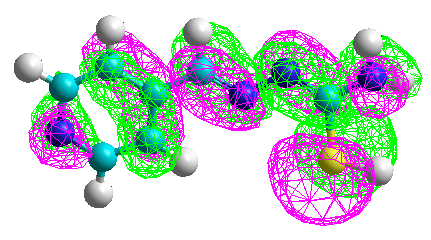
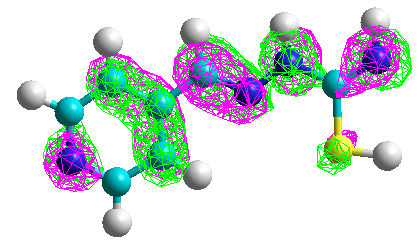
Electrostatic Potential

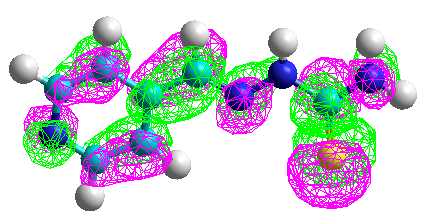
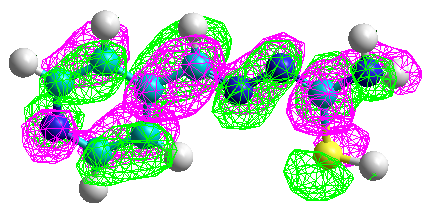
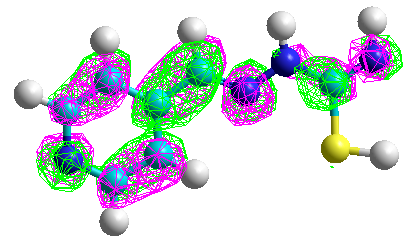
Total Spin Density

Total Charge Density

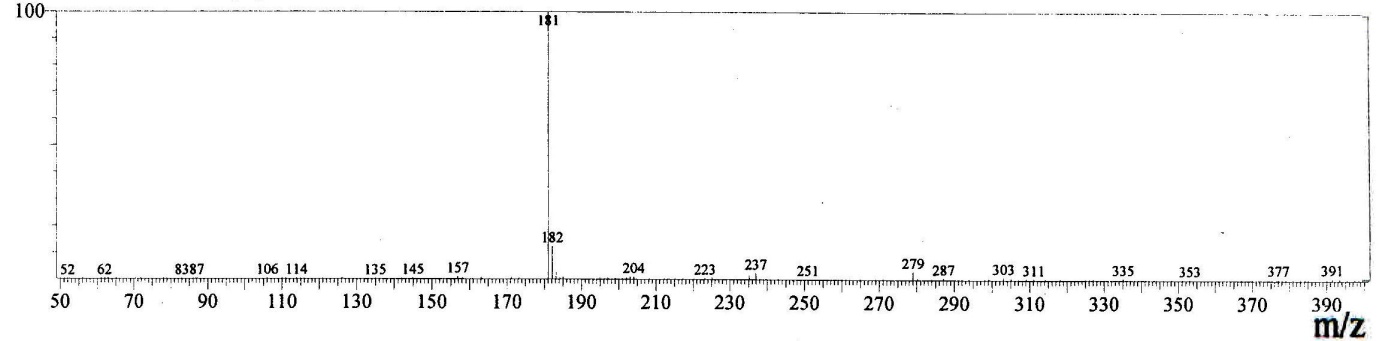
  

Highest Occupied Molecular Orbital

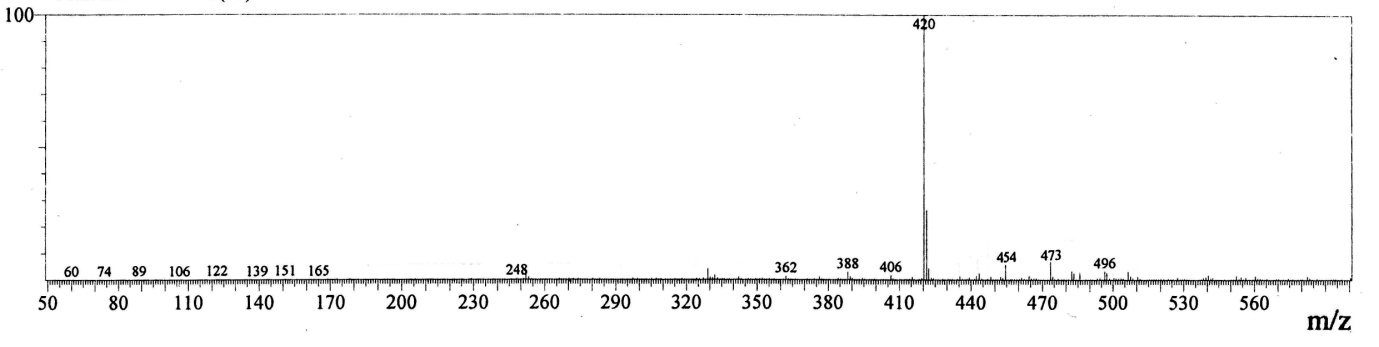
  

Lowest Unoccupied Molecular Orbital

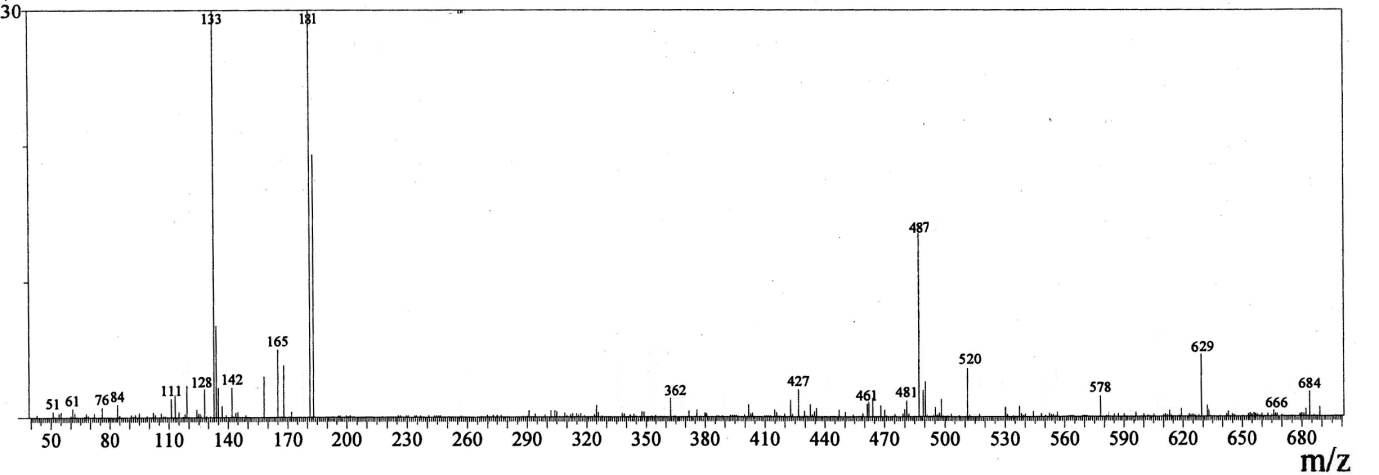
Figure S1. Molecular Graphs of H4FPT (L)

****

a. H4FPT (L)

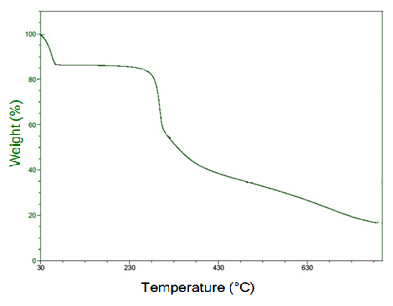
****

b. Ni(II) complex

****

c. Cu(II) complex

Figure S2.Mass spectra of H4FPT, Ni(II) and Cu(II) complexes

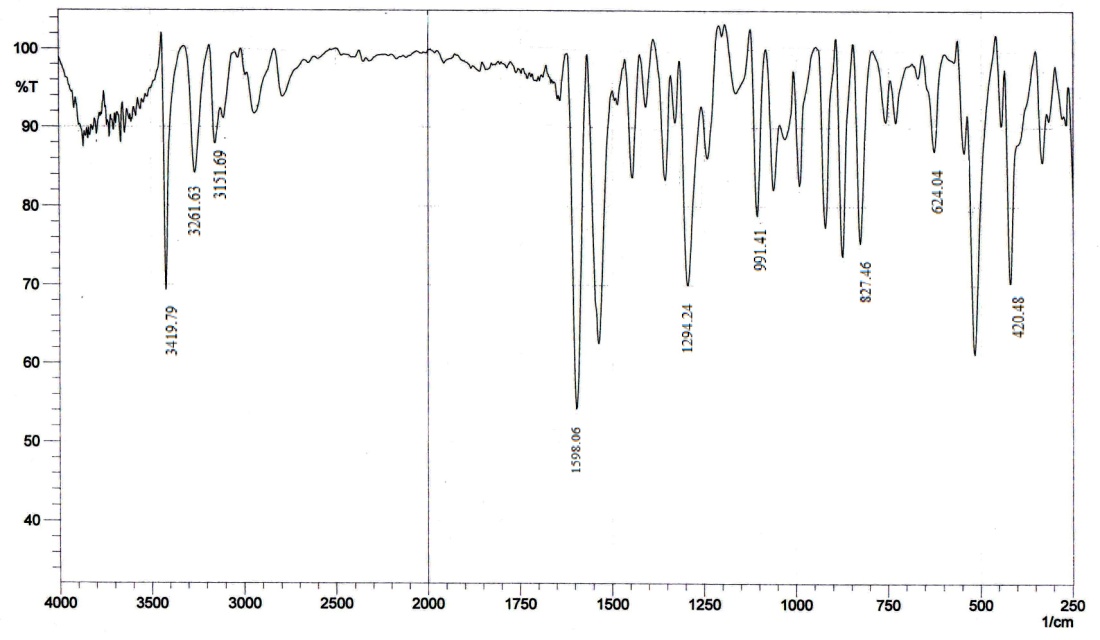


a. Ni(II) complex

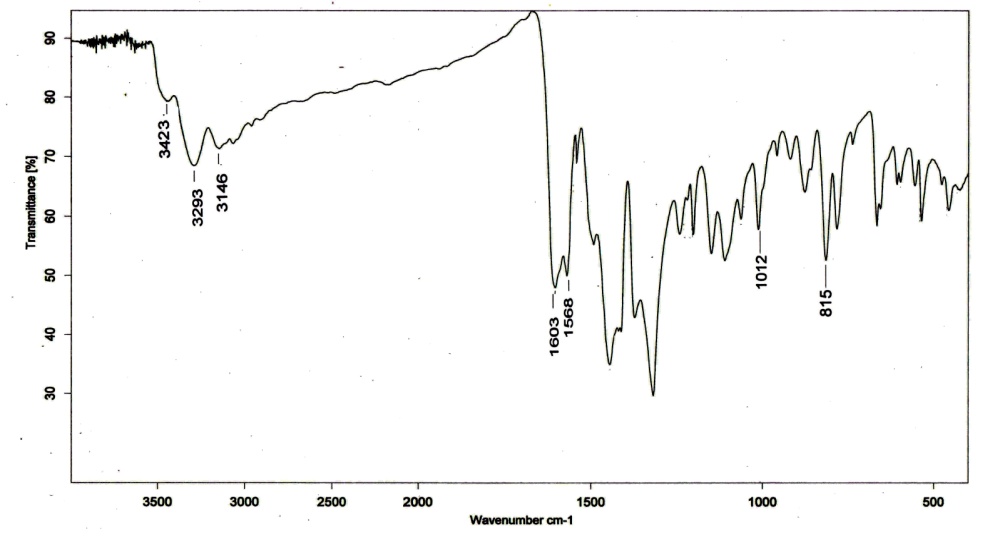


b. Cu(II) complex

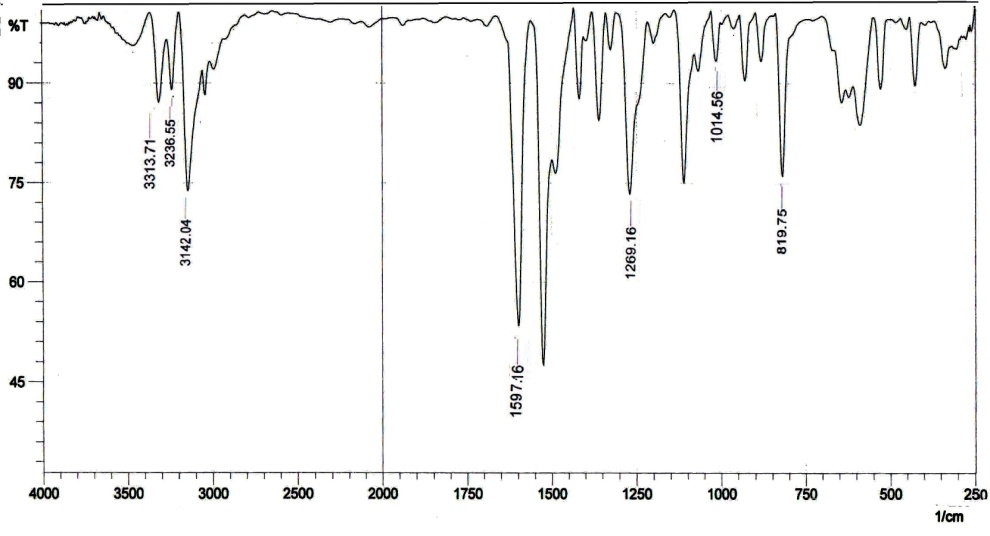
Figure S3.Thermograms of Ni(II) and Cu(II) complexes



a. H4FPT (L)

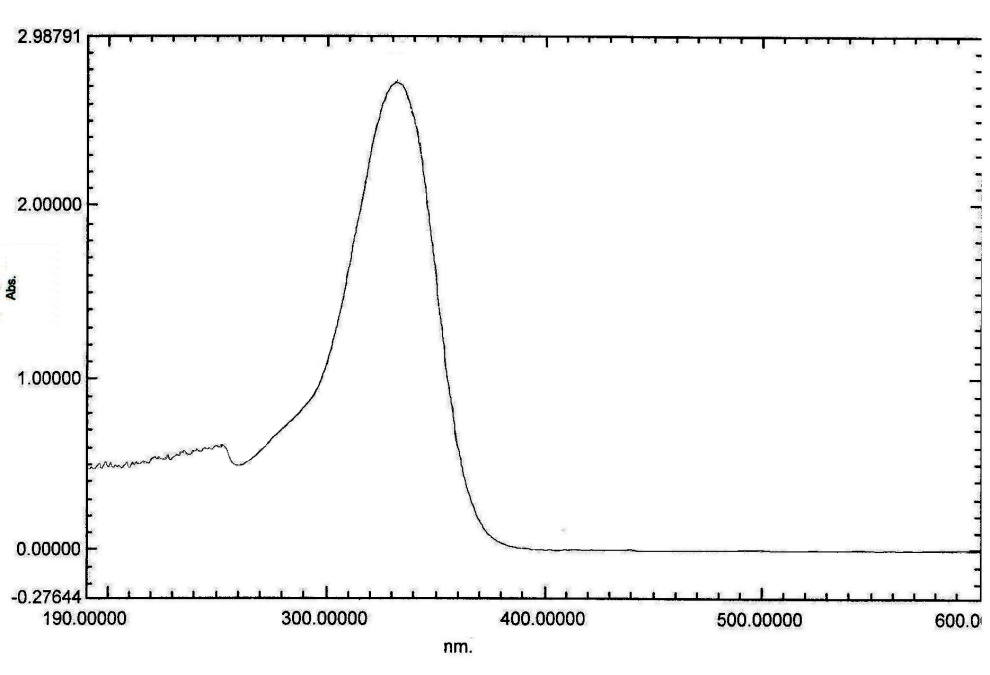


b. Ni(II) complex

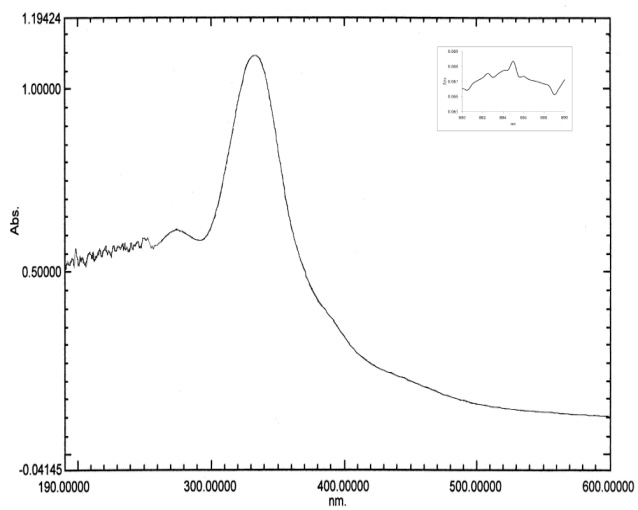


c. Cu(II) complex

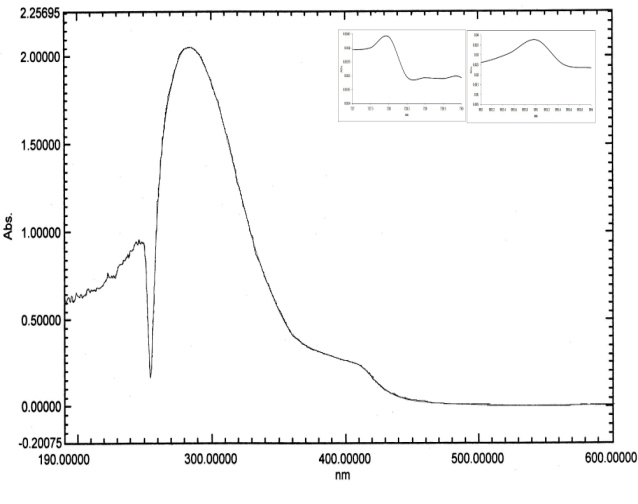
Figure S4.IR Spectra of H4FPT, Ni(II) and Cu(II) complexes



a. H4FPT (L)



b. Ni(II) complex

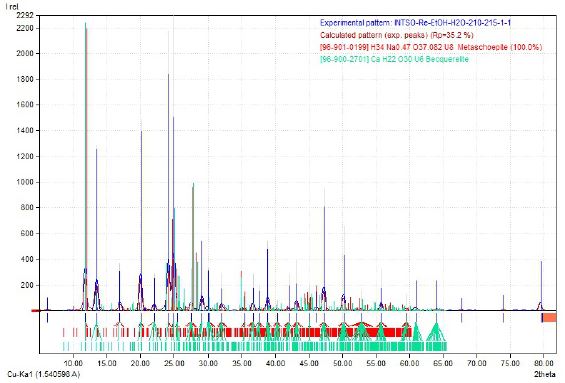


c. Cu(II) complex

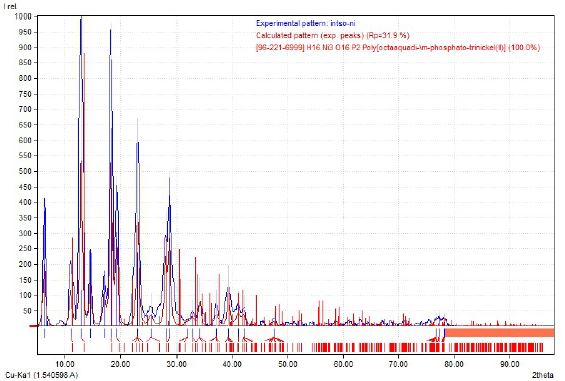
Figure S5.UV-Visible Spectra of H4FPT, Ni(II) and Cu(II) complexes



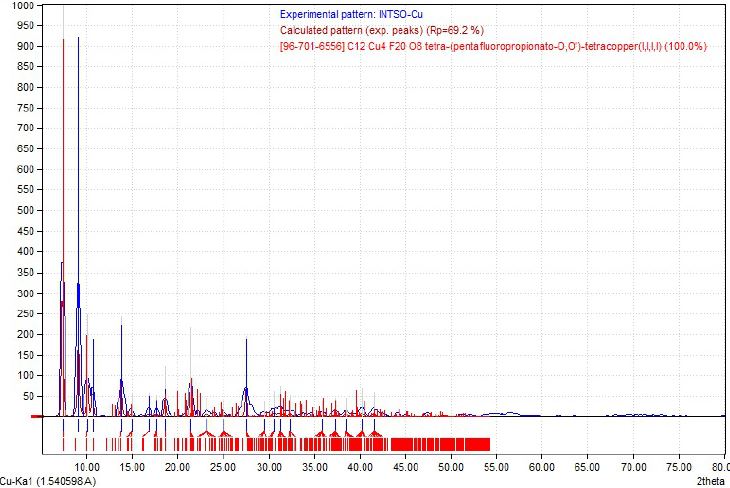
Figure S6.ESR spectra of Cu(II) complex



a. H4FPT (L)

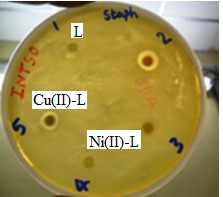
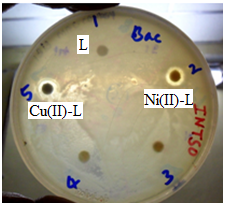


b. Ni(II) complex

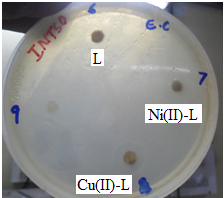
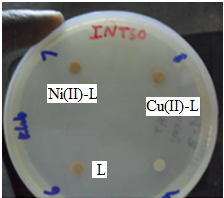


c. Cu(II) complex

Figure S7.Powder XRD of H4FPT, Ni(II) and Cu(II) complexes

a) *S.aureus* b) *B.subtilis*

c) *E.coli* d) *K.pneumoniae*

Figure S8.Antibacterial activity of H4FPT (L) and its Ni(II) and Cu(II) complexes

with zone of inhibition in mm

Table S1: Data showing decrease in fluorescence emission with increase in concentration of the Ni(II)- H4FPTcomplex

|  |  |  |  |
| --- | --- | --- | --- |
| Concentration of the complex x10-6 M | % increase in Concentration | Intensity of emission | % decrease in Intensity |
| 0.78 | 96.85 | 81.88 | 1.78 |
| 1.55 | 47.74 | 80.43 | 1.25 |
| 2.29 | 31.35 | 79.42 | 3.81 |
| 3.01 | 23.14 | 76.39 | 1.79 |
| 3.70 | 18.25 | 75.03 | 1.08 |
| 4.38 | 14.98 | 74.22 | 1.35 |
| 5.04 | 12.67 | 73.22 | 1.20 |
| 5.67 | 10.93 | 70.14 | 3.10 |
| 6.29 | 9.58 | 70.04 | 0.08 |

Table S2: Data showing decrease in fluorescence emission with increase in concentration of the Cu(II)- H4FPTcomplex

|  |  |  |  |
| --- | --- | --- | --- |
| Concentration of the complex x10-6 M | Increase in % Concentration | Intensity of emission | Decrease in % Intensity |
| 0.78 | 96.85 | 77.12 | 0.26 |
| 1.55 | 47.74 | 76.92 | 2.03 |
| 2.29 | 31.35 | 75.35 | 2.35 |
| 3.01 | 23.14 | 73.58 | 1.68 |
| 3.70 | 18.25 | 72.34 | 1.23 |
| 4.38 | 14.98 | 71.46 | 2.69 |
| 5.04 | 12.67 | 69.53 | 1.16 |
| 5.67 | 10.93 | 68.74 | 1.14 |
| 6.29 | 9.58 | 67.94 | 1.96 |