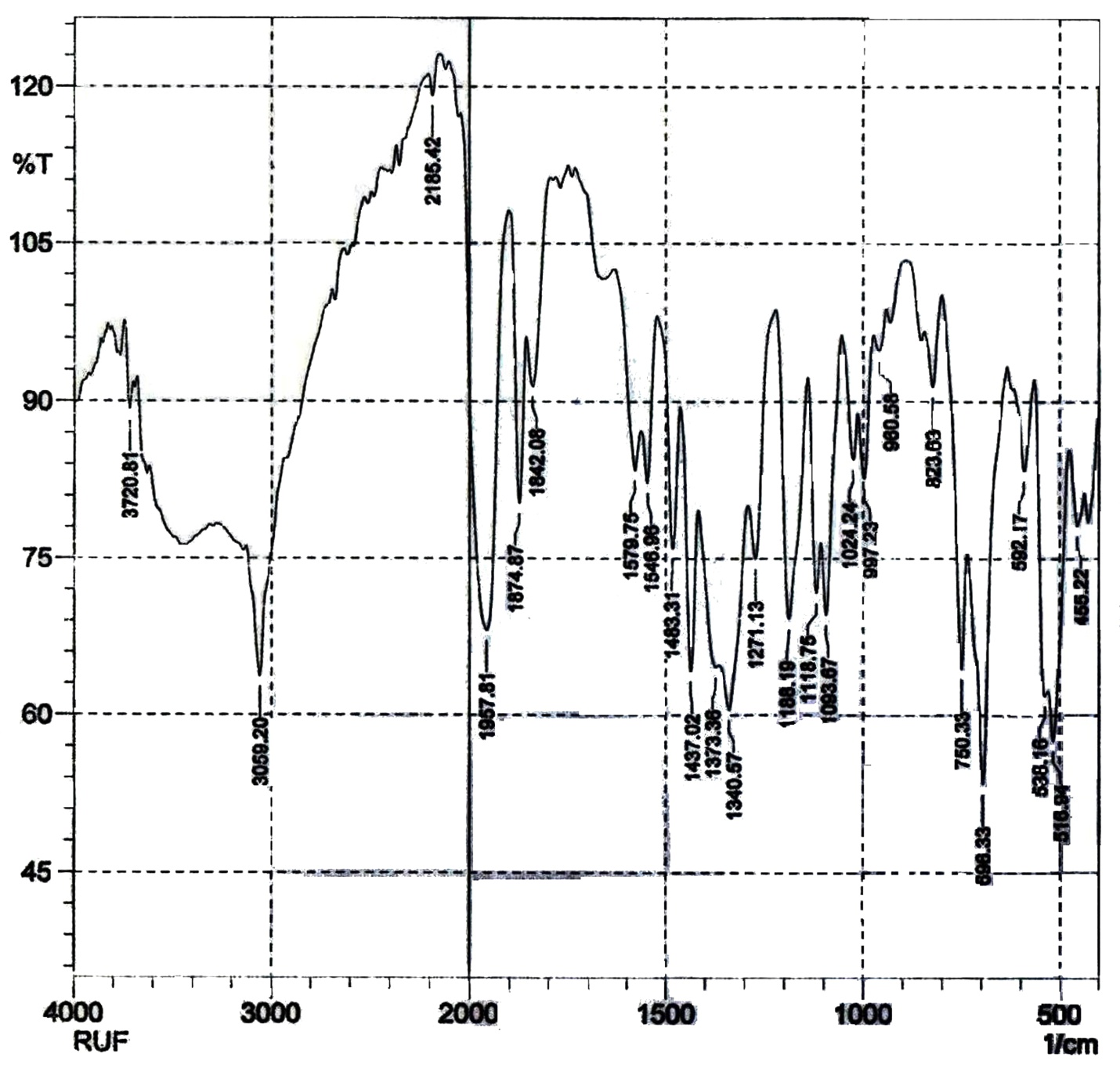
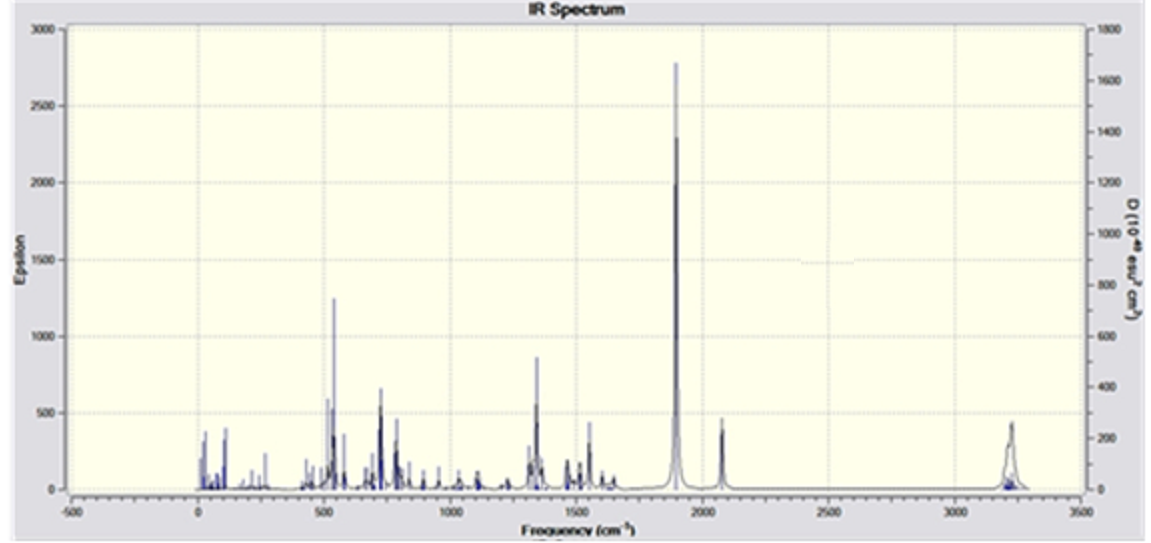
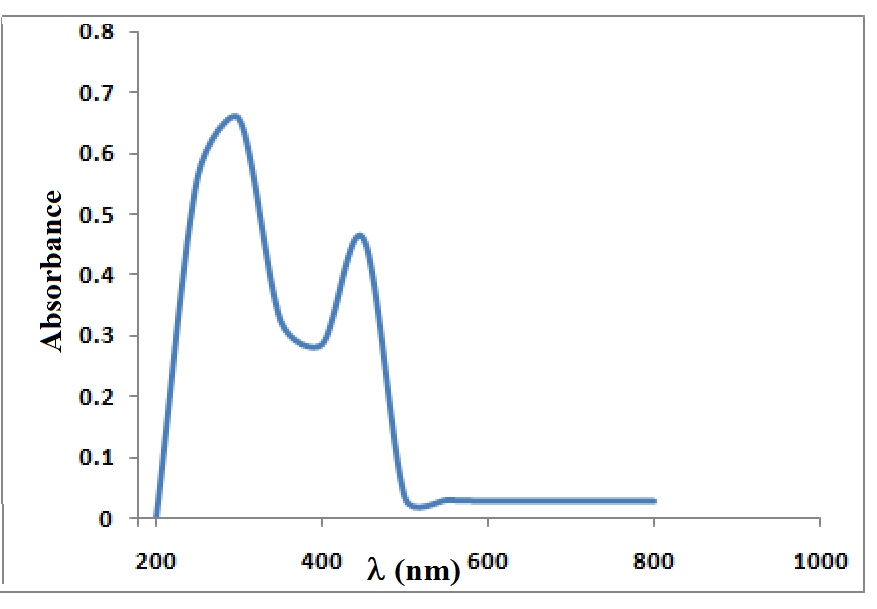
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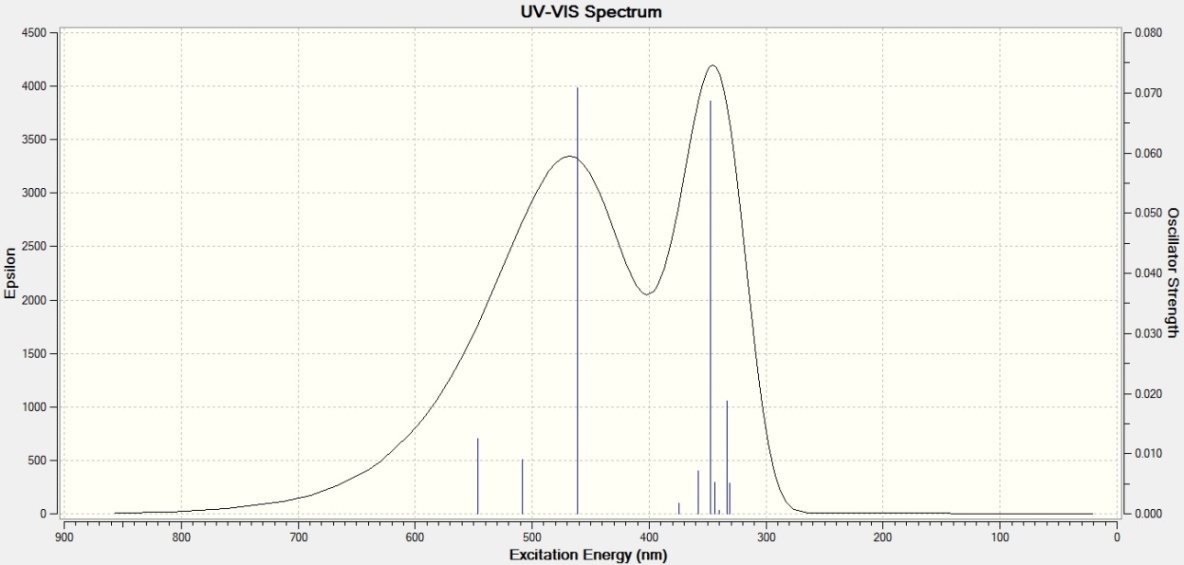
**Fig. S1.** ExperimentalFTIR Spectrum of the [RuHCl(CO)(bpy)(tpp)] complex



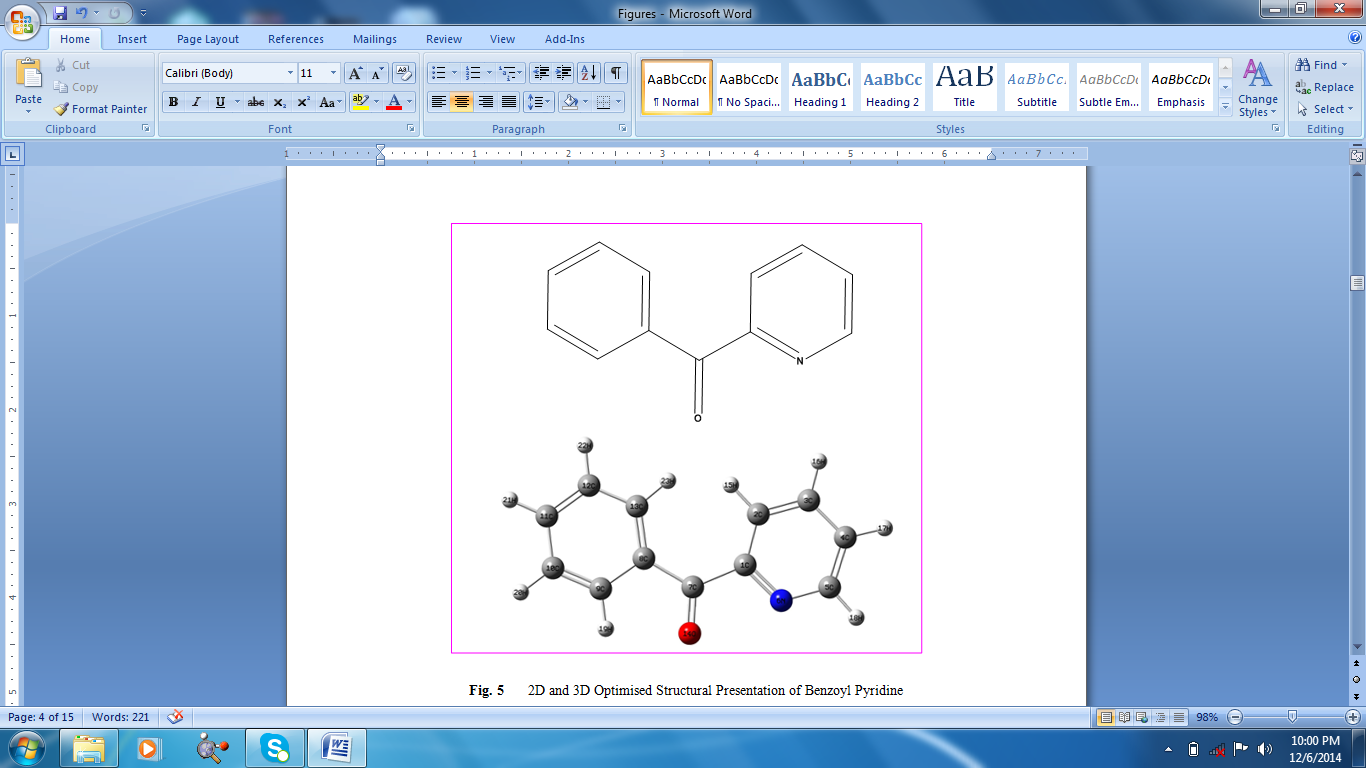
**Fig. S2.** TheoreticalFTIR Spectrum of the complex



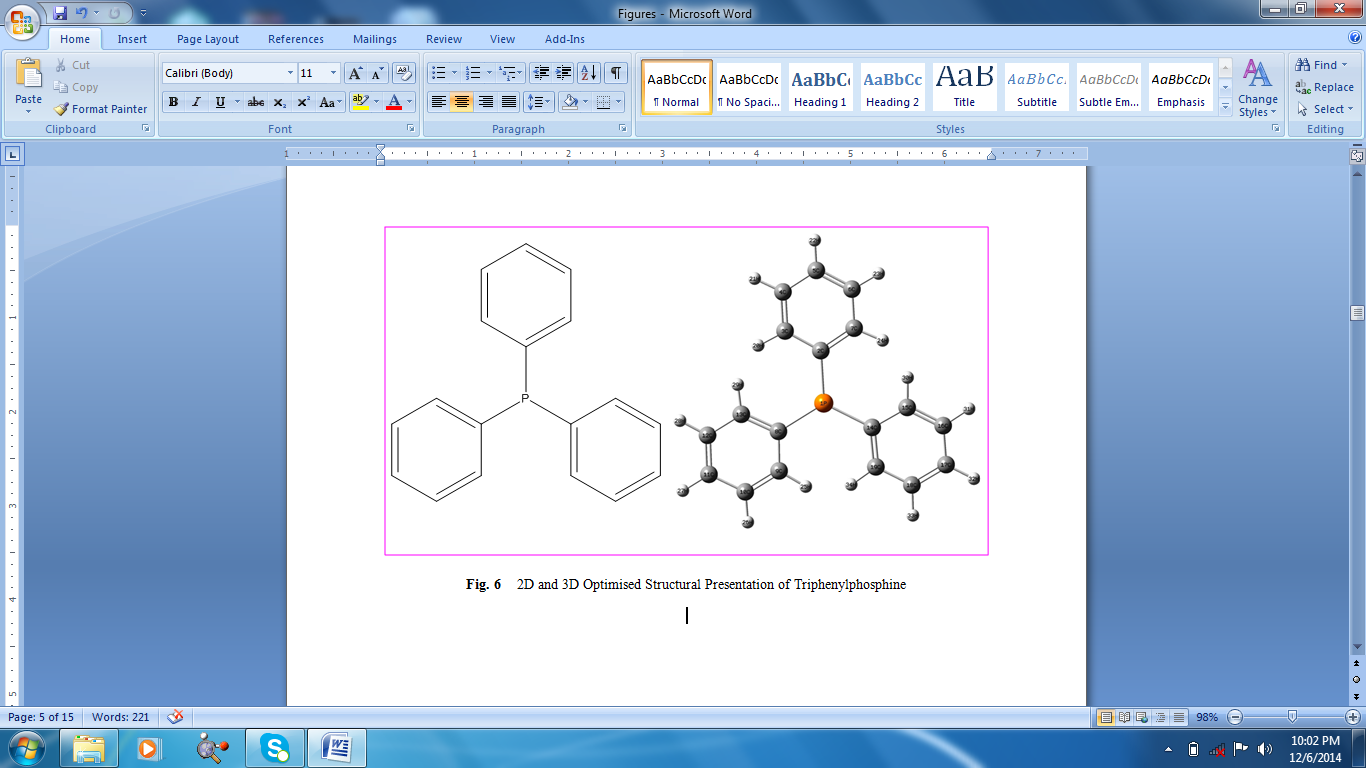
**Fig. S3.** Experimental UV-Visible spectrum of [RuHCl(CO)(bpy)(tpp)] Complex



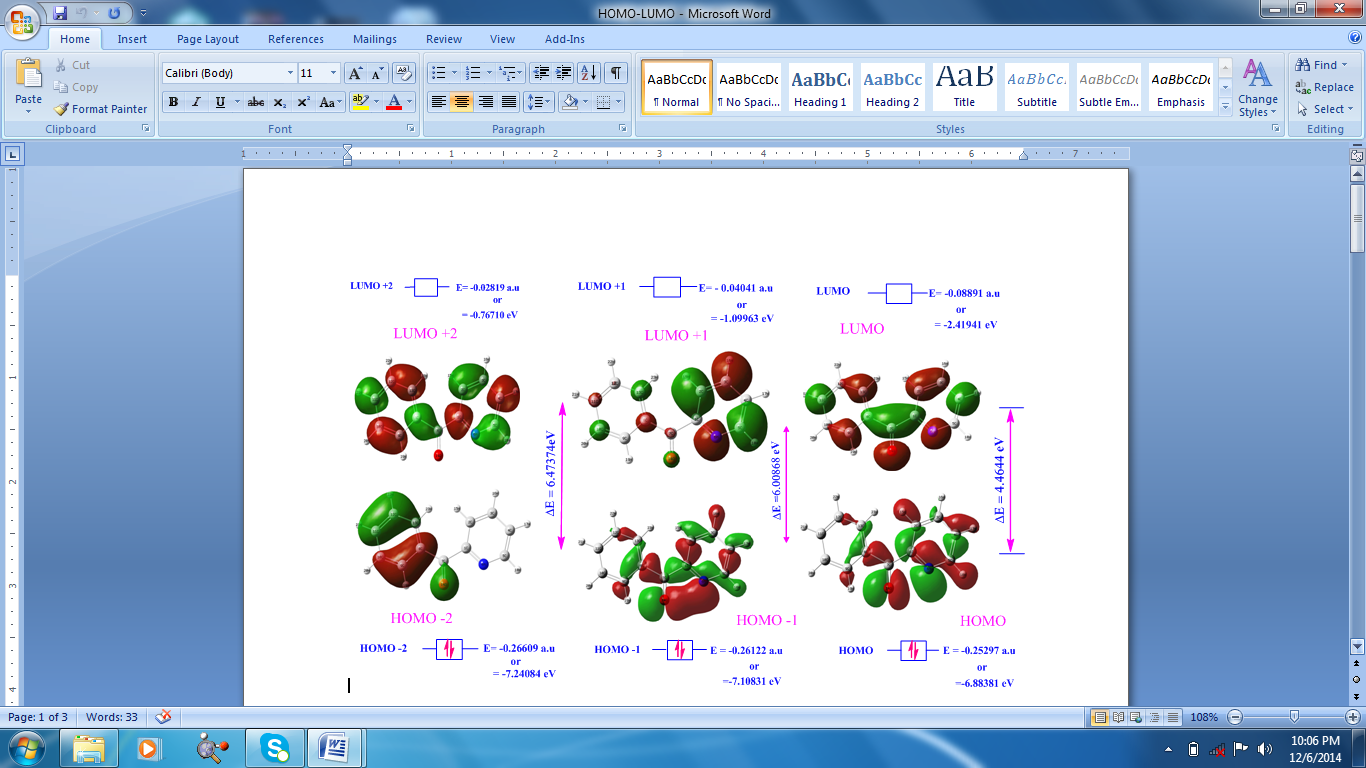
**Fig. S4.** TD-DFT UV-Vis Spectrum of [RuHCl(CO)(bpy)(tpp)] Complex

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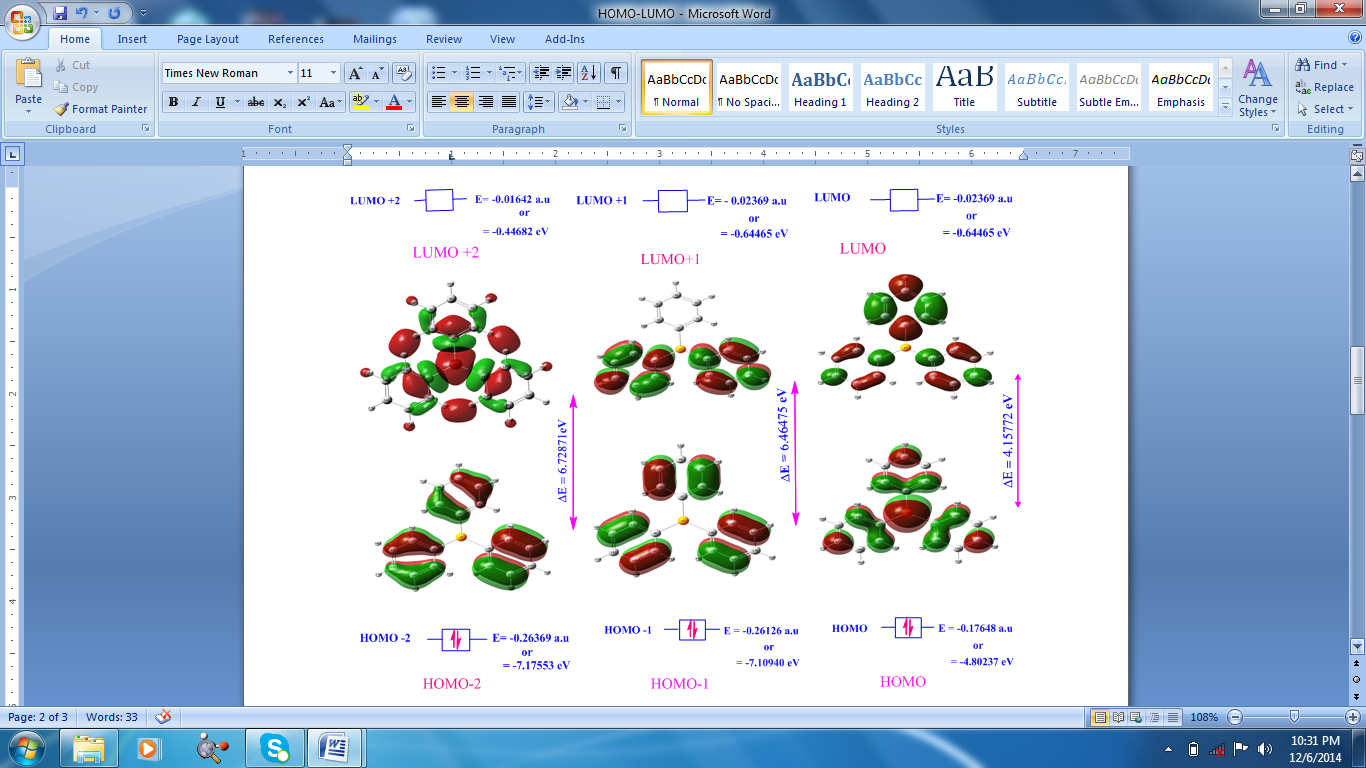
**Fig. S5.** 2D and 3D optimized structural presentation of benzoylpyridine

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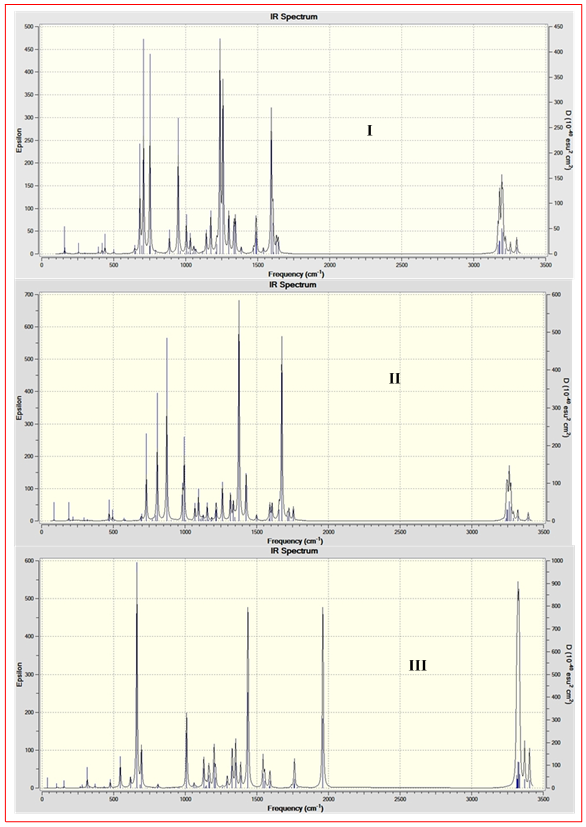
**Fig. S6.** 2D and 3D Optimized structural presentation of Triphenylphosphine

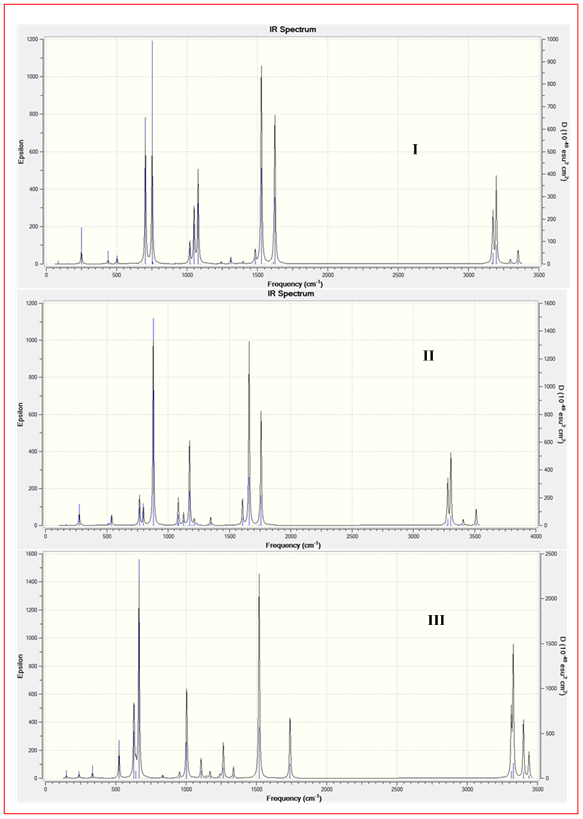


**Fig. S7**. HOMO-LUMO structure with energy level diagram of benzoyl pyridine ligand



**Fig. S8** HOMO-LUMO structure with energy level diagram of Triphenylphosphine ligand



**Fig.** **S9.**  DFT based IR Spectrum of benzoylpyridine based 

**Fig. S10.**  DFT based IR Spectrum of Tpp ligand

Table S1: Antiproliferative data of the compounds

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| S. No. | Sample | Absorbance by control | Concentration of sample (μg/mL) | Absorbance by sample | Cell Survival (%) | Cell Death  (%) |
| 1 | [Ru(CO)(H)(Cl)(Tpp)3 | 1.22 | 10 | 0.193 | 84.18 | 33.85 |
|  | IC50= 53 |  | 20 | 0.287 | 76.47 | 41.55 |
|  |  |  | 40 | 0.343 | 71.88 | 46.14 |
|  |  |  | 80 | 0.541 | 55.65 | 62.37 |
| 2 | [Ru(CO)(H)(Cl)(Bpy)(Tpp) | 1.94 | 10 | 0.211 | 89.12 | 59.33 |
|  | IC50= 40 |  | 20 | 0.343 | 82.32 | 66.13 |
|  |  |  | 40 | 0.383 | 80.26 | 68.19 |
|  |  |  | 80 | 0.508 | 73.81 | 74.64 |