

Supplementary Material:

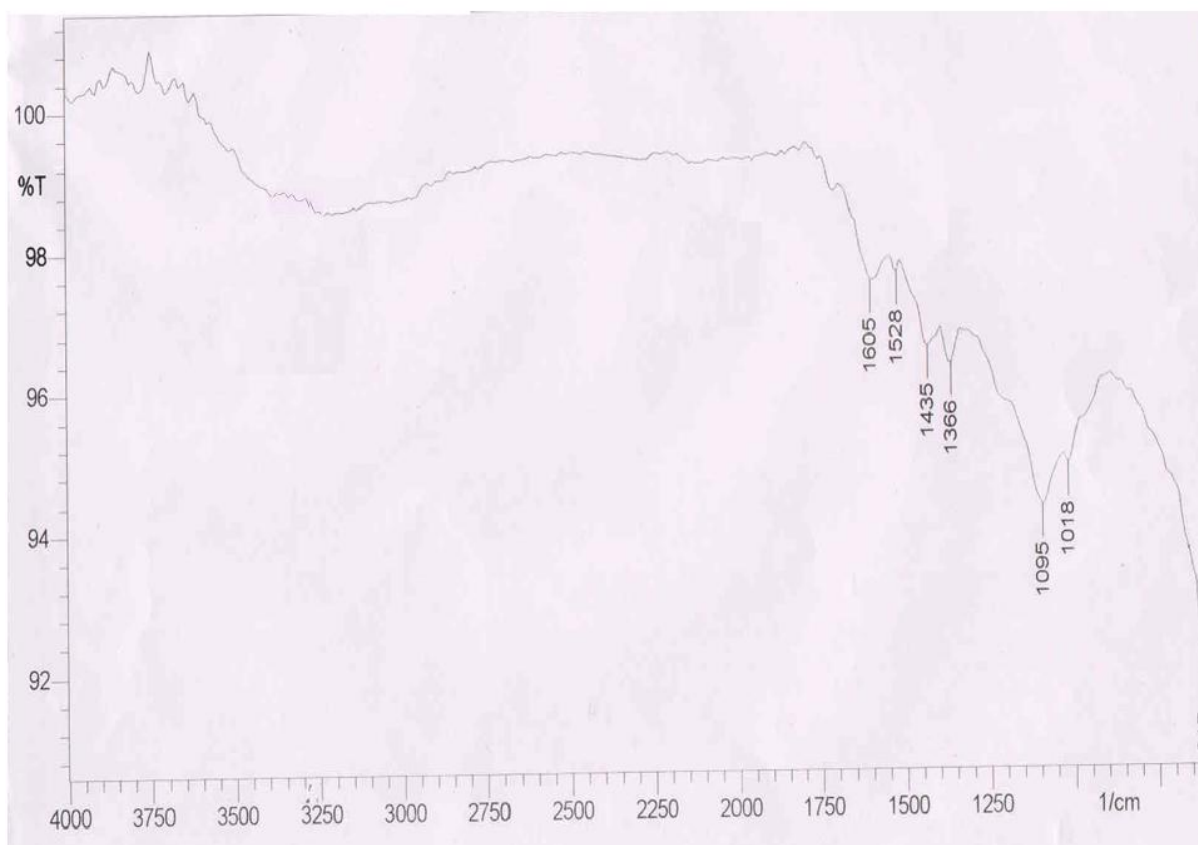


Figure: S1(a) IR Spectrum of [Cr (C₃₆H₃₆N₄) Cl] Cl₂

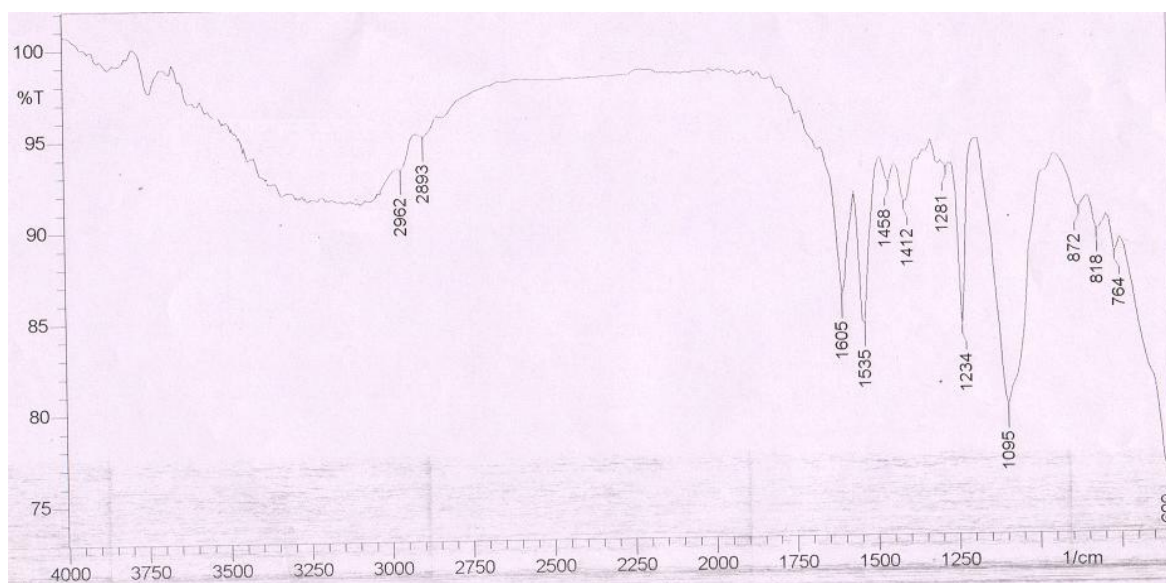


Figure: S1(b) IR Spectrum of [Cr (C₃₆H₃₆N₄) NO₃] (NO₃)₂



Figure: S1(c) IR Spectrum of $[\text{Cr} (\text{C}_{36}\text{H}_{36}\text{N}_4) (\text{OAc})] (\text{OAc})_2$

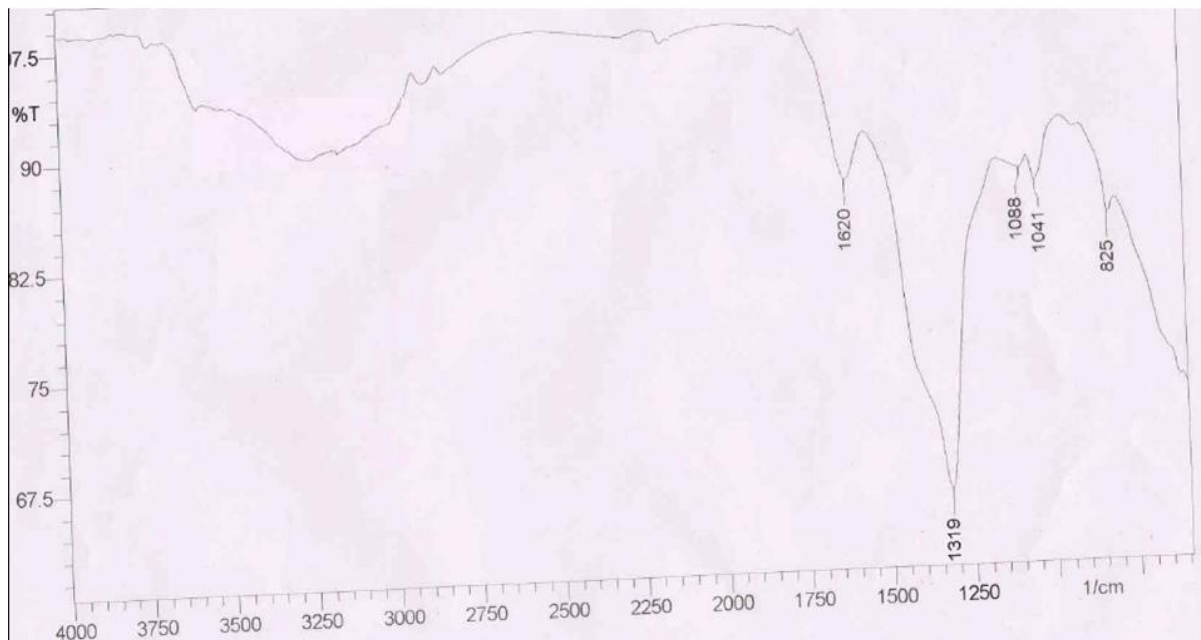


Figure: S1(d) IR Spectrum of $[\text{Fe} (\text{C}_{36}\text{H}_{36}\text{N}_4) \text{Cl}] \text{Cl}_2$

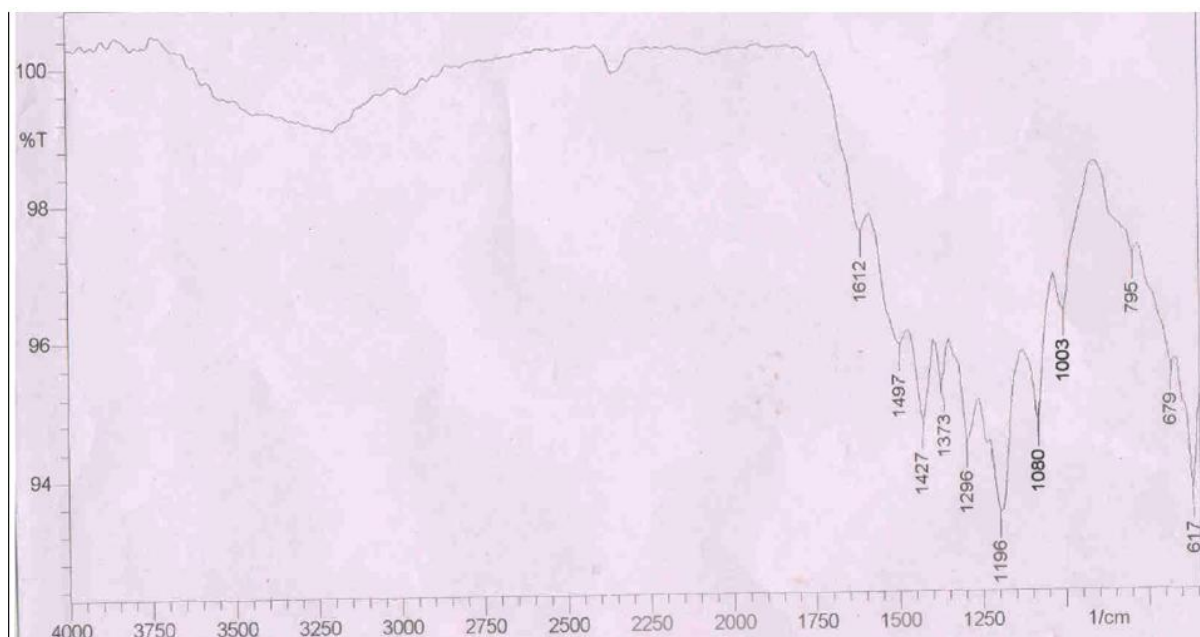
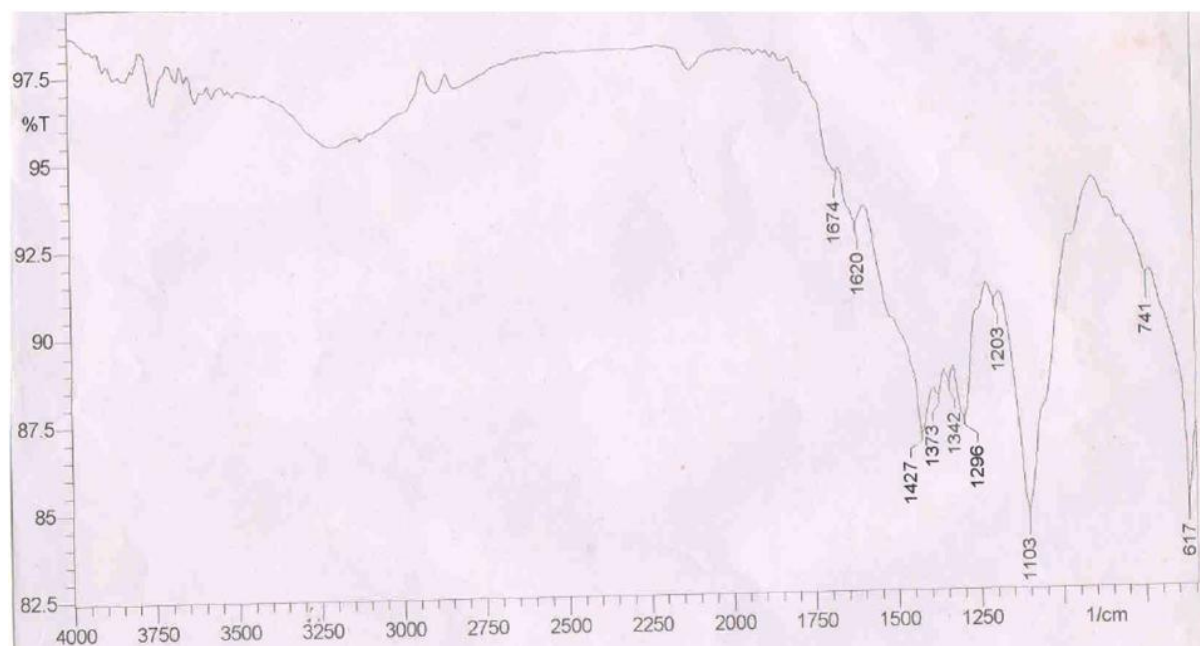


Figure: S1(e) IR Spectrum of $[\text{Fe}(\text{C}_{36}\text{H}_{36}\text{N}_4)\text{NO}_3](\text{NO}_3)_2$



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Figure: S1(f) IR Spectrum of $[\text{Fe}(\text{C}_{36}\text{H}_{36}\text{N}_4)(\text{OAc})](\text{OAc})_2$

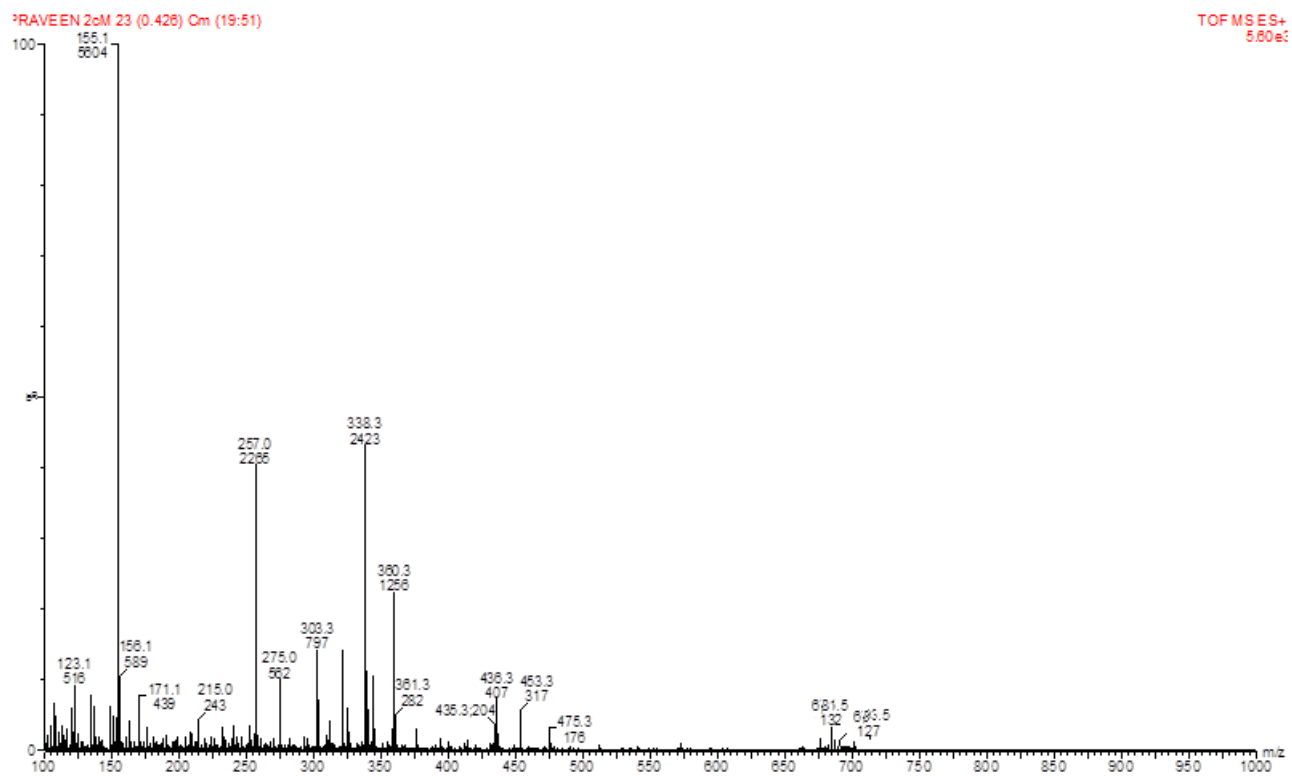


Figure: S2 Mass Spectrum of $[\text{Cr}(\text{C}_{36}\text{H}_{36}\text{N}_4)\text{Cl}](\text{Cl})_2$

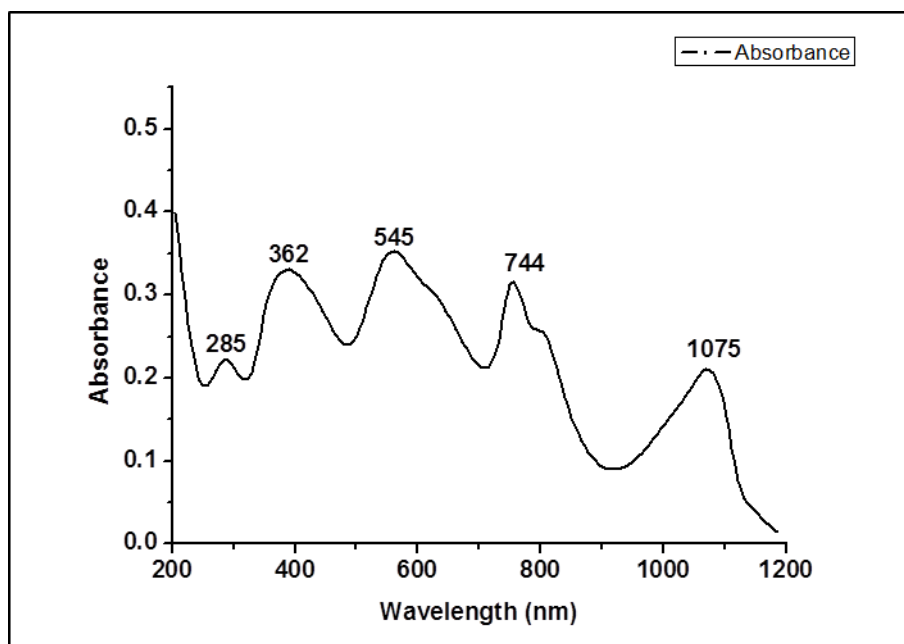


Figure: S3(a) Electronic Spectra of [Cr (C₃₆H₃₆N₄) Cl] Cl₂

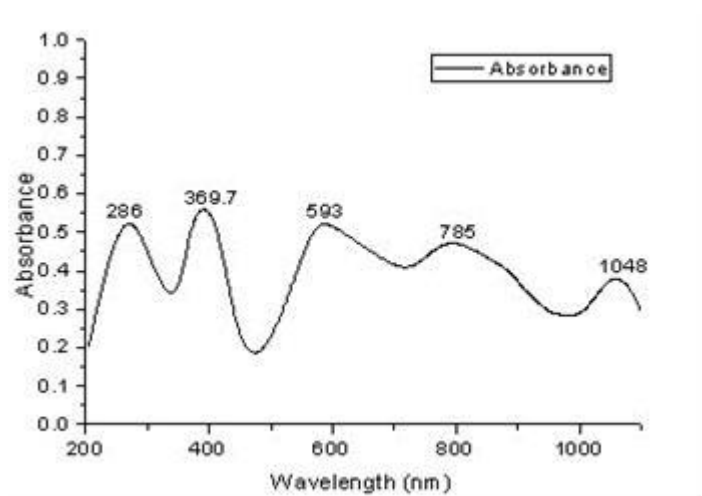


Figure: S3(b) Electronic Spectra of [Cr (C₃₆H₃₆N₄) NO₃] (NO₃)₂

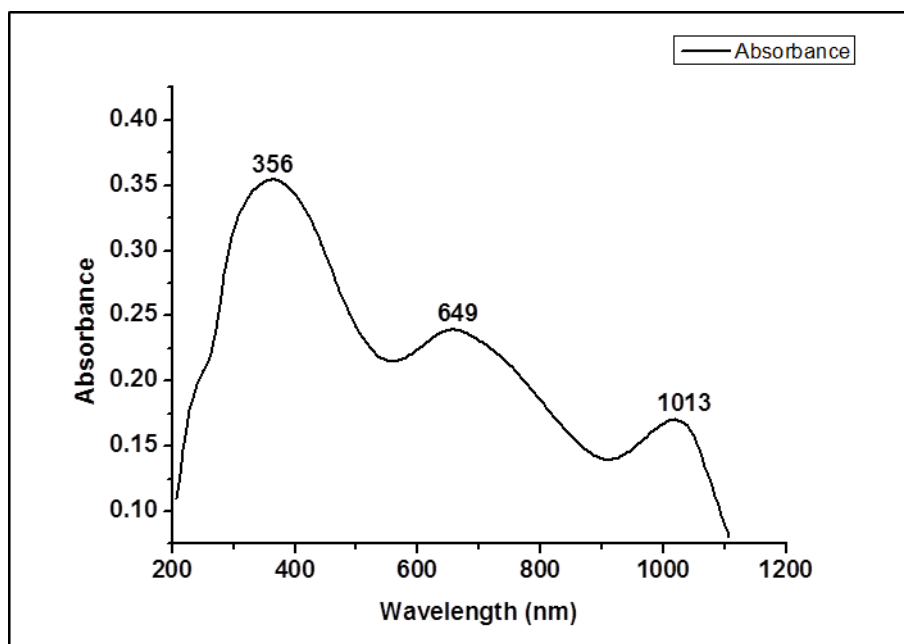


Figure: S3(c) Electronic Spectra of [Fe (C₃₆H₃₆N₄) Cl] Cl₂

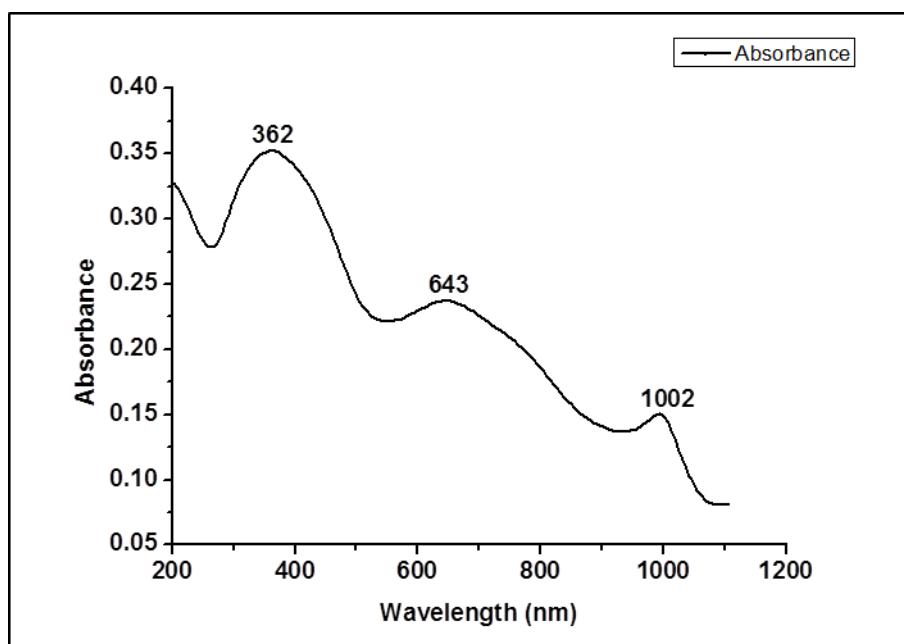


Figure: S3(d) Electronic Spectra of [Fe (C₃₆H₃₆N₄) NO₃] (NO₃)₂

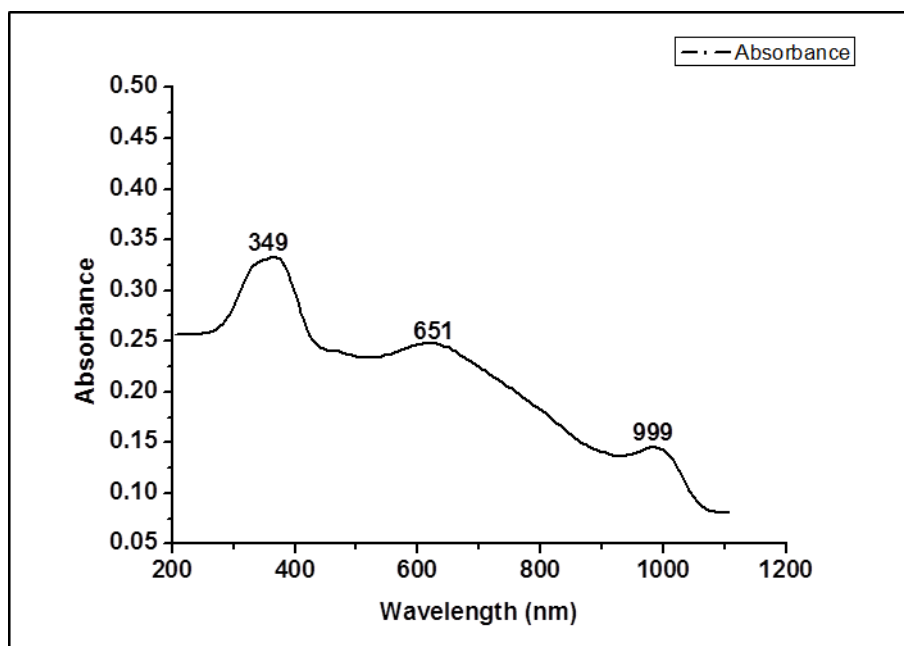


Figure: S3(e) Electronic Spectra of [Fe (C₃₆H₃₆N₄) (OAc)] (OAc)₂

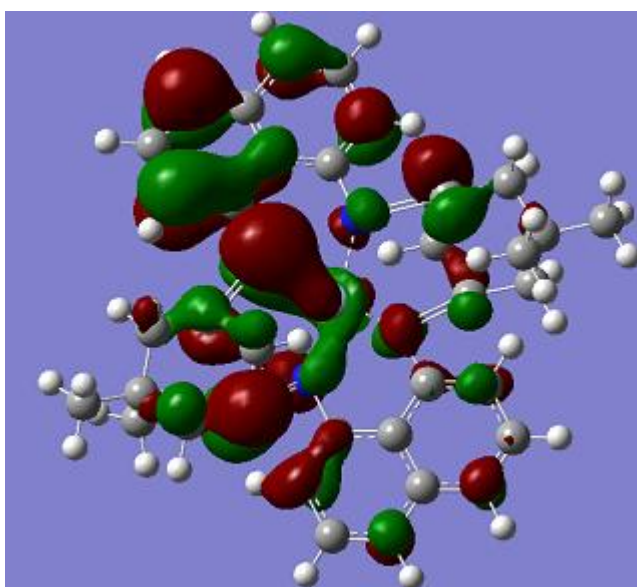
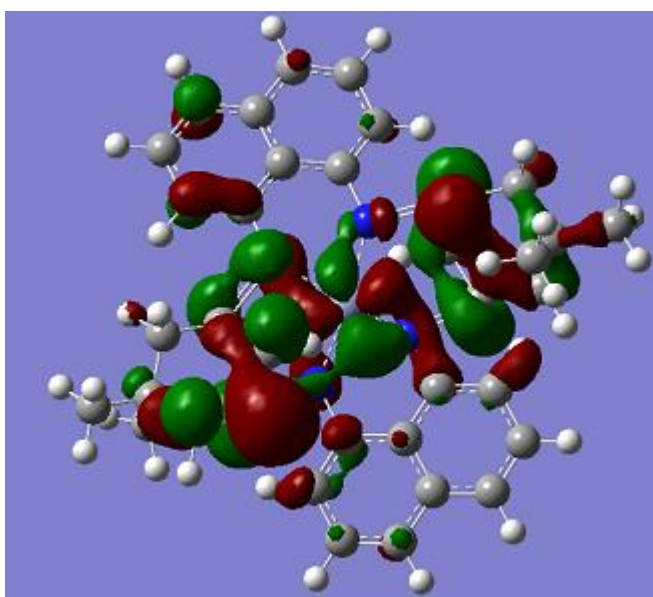


Figure: S4 HOMO-LUMO orbitals of B3LYP geometry optimized structure of [Cr (C₃₆H₃₆N₄) Cl] (Cl)₂

Supplementary Material Figure Captions:

Figure: S1(a) IR Spectrum of [Cr (C₃₆H₃₆N₄) Cl] Cl₂

Figure: S1(b) IR Spectrum of [Cr (C₃₆H₃₆N₄) NO₃] (NO₃)₂

Figure: S1(c) IR Spectrum of [Cr (C₃₆H₃₆N₄) (OAc)] (OAc)₂

Figure: S1(d) IR Spectrum of [Fe (C₃₆H₃₆N₄) Cl] Cl₂

Figure: S1(e) IR Spectrum of [Fe (C₃₆H₃₆N₄) NO₃] (NO₃)₂

Figure: S1(f) IR Spectrum of [Fe (C₃₆H₃₆N₄) (OAc)] (OAc)₂

Figure: S2 Mass Spectrum of [Cr (C₃₆H₃₆N₄) Cl] (Cl)₂

Figure: S3(a) Electronic Spectra of [Cr (C₃₆H₃₆N₄) Cl] Cl₂

Figure: S3(b) Electronic Spectra of [Cr (C₃₆H₃₆N₄) NO₃] (NO₃)₂

Figure: S3(c) Electronic Spectra of [Fe (C₃₆H₃₆N₄) Cl] Cl₂

Figure: S3(d) Electronic Spectra of [Fe (C₃₆H₃₆N₄) NO₃] (NO₃)₂

Figure: S3(e) Electronic Spectra of [Fe (C₃₆H₃₆N₄) (OAc)] (OAc)₂

Figure: S4 HOMO-LUMO orbitals of B3LYP geometry optimized structure of [Cr (C₃₆H₃₆N₄) Cl] (Cl)₂