Insight into the synthesis, structure affirmation and catalytic efficiency of divalent and trivalent metal chelates of mandelic acid hydrazone derivative

Hoda A. El-Ghamry[1]*, Mohamed Gaber[1], Fatmah M Alkhatib[2], Hossa F. Al Shareef[2], Khadiga M. Takroni[2], Shaimaa K. Fathalla[3]

[1]Chemistry Department, Faculty of Science, Tanta University, Tanta, Egypt

[2]Chemistry Department, Faculty of Applied Science, Umm Al-Qura University, Saudi Arabia

[3]Chemistry Department, Faculty of Science, Taif University, Taif, Saudi Arabia

* Corresponding author email: hoda.elghamri@science.tanta.edu.eg

Section S1 Catalytic oxidation of o-aminophenol (OAP)

The phenoxazinone synthase like efficacy of the synthesized chelates have been evaluated by utilizing o-aminophenol (OAP) as the paradigm substrate in dimethyl formamide medium at room temperature. For this study, $3x10^{-5}$ M solution of each complex have been firstly treated with 10^{-2} M of the substrate o-aminophenol under aerobic environment. The catalytic reactions have been followed up by the UV-Vis spectral recording of the increase in the absorbance peak of the product 2-amino-phenoxazine-3-one (APX) in the range 430-435 nm upon mixing as a function of time at 5 min time intervals this is up to ≈ 80 minutes. The initial rate method was used to determine the rate of reaction from the slope of the absorbance against time plot in the liner region [1]. The initial rate has been calculated using 18300 M^{-1} cm^{-1} as the molar absorptivity of the product 2-aminobenzoxazine-3-one [2, 3].

Kinetics of OAP oxidation were studied and explained by observation and recording the increase of phenoxazinone spectral band at 431 nm. The investigated materials under interest illustrated saturation kinetics, and the obtained results were treated applying the Michaelis-Menten model which looks suitable for the obtained results. The Michaelis constant (K_M, M), maximum reaction velocity (Vmax, M min^{-1}),

specificity constant (k_{cat}/K_M in M^{-1} h^{-1}). and rate constant for substrates dissociation (i.e. turnover number; k_{cat}, h^{-1}) were calculated for all synthesized compounds.

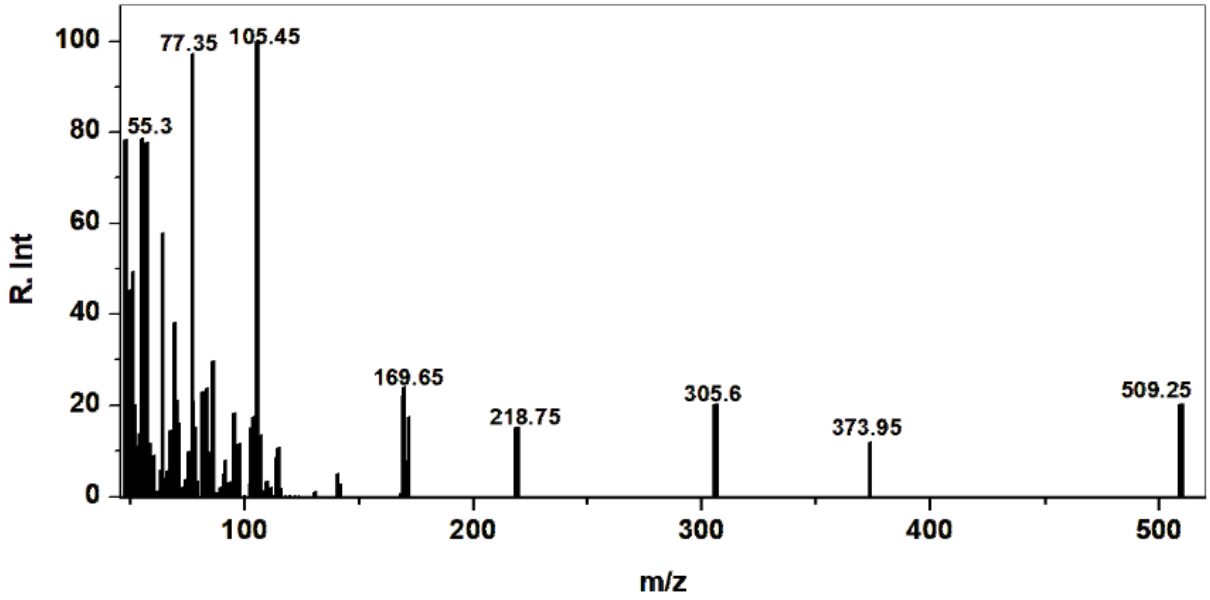

Fig. S1. Mass spectra of **PANH-Cr** chelate

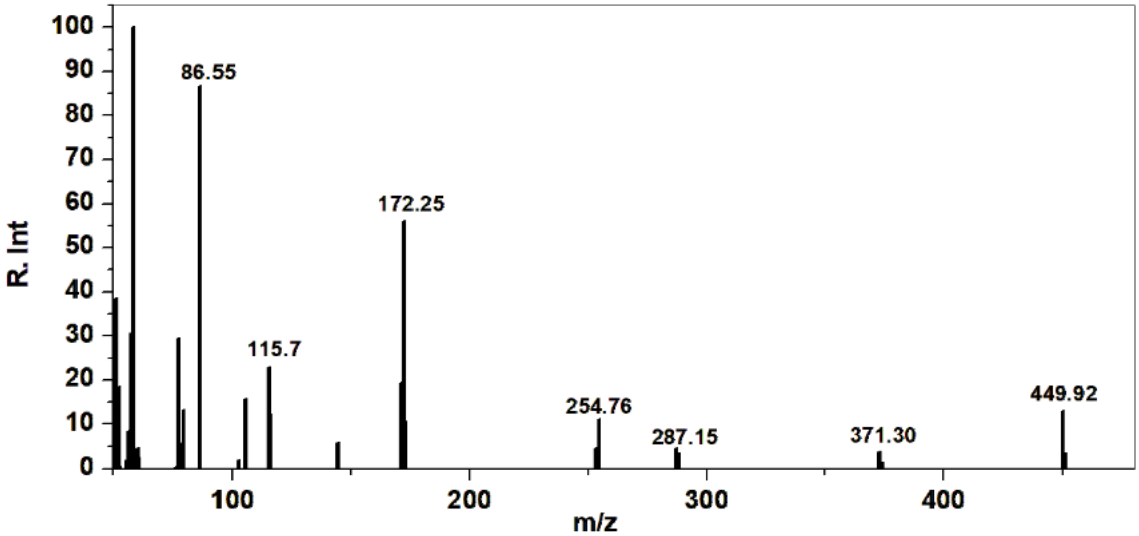

Fig. S2. Mass spectra of **PANH-Co** chelate

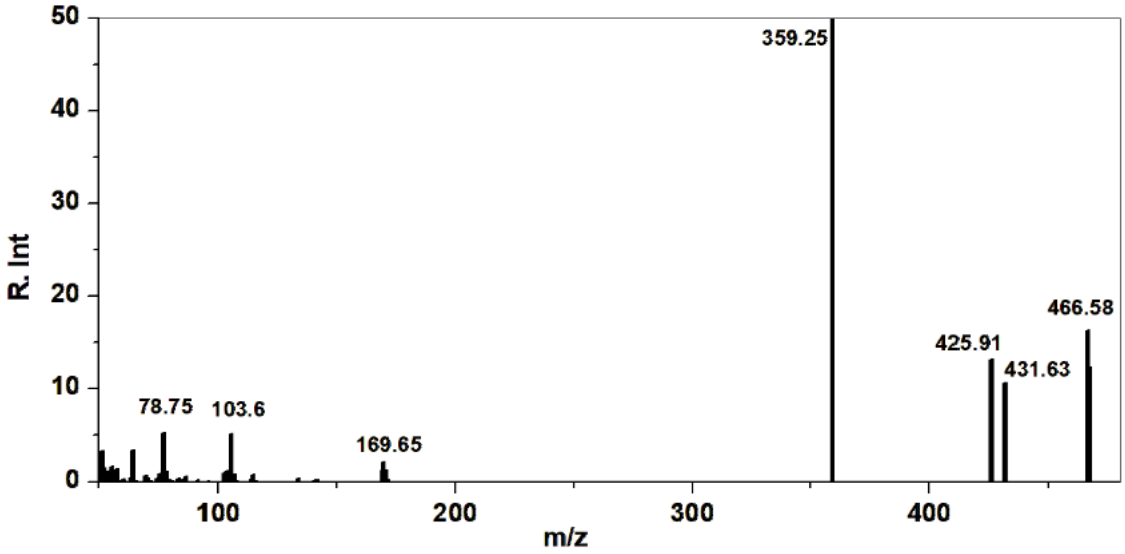

Fig. S3. Mass spectra of **PANH-Ni** chelate

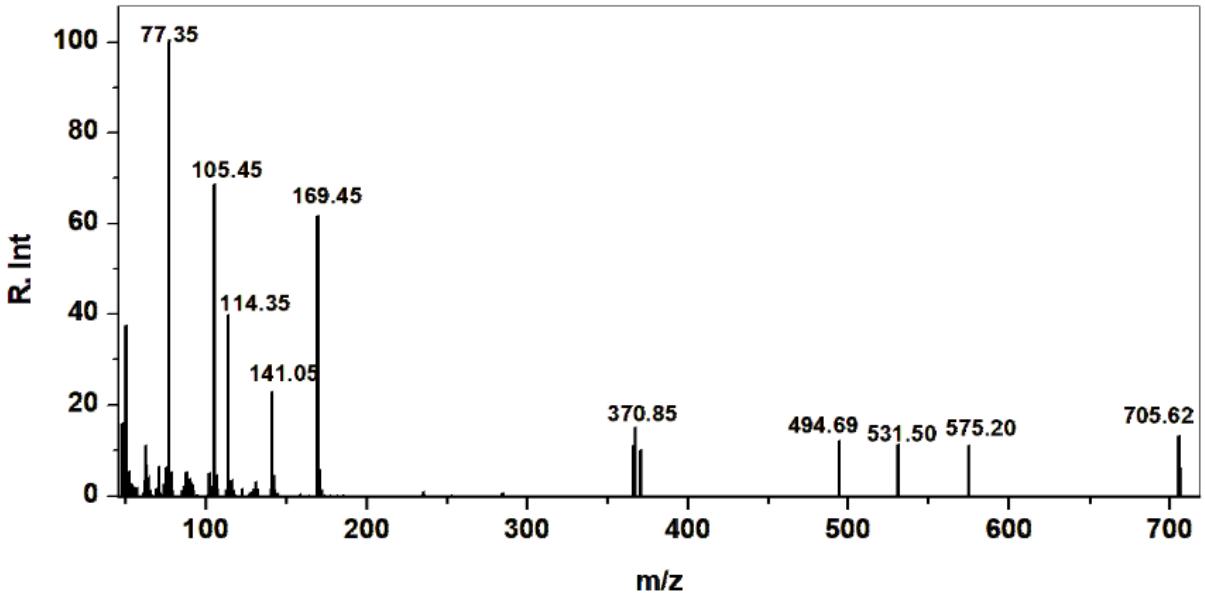

Fig. S4. Mass spectra of **PANH-Cu** chelate

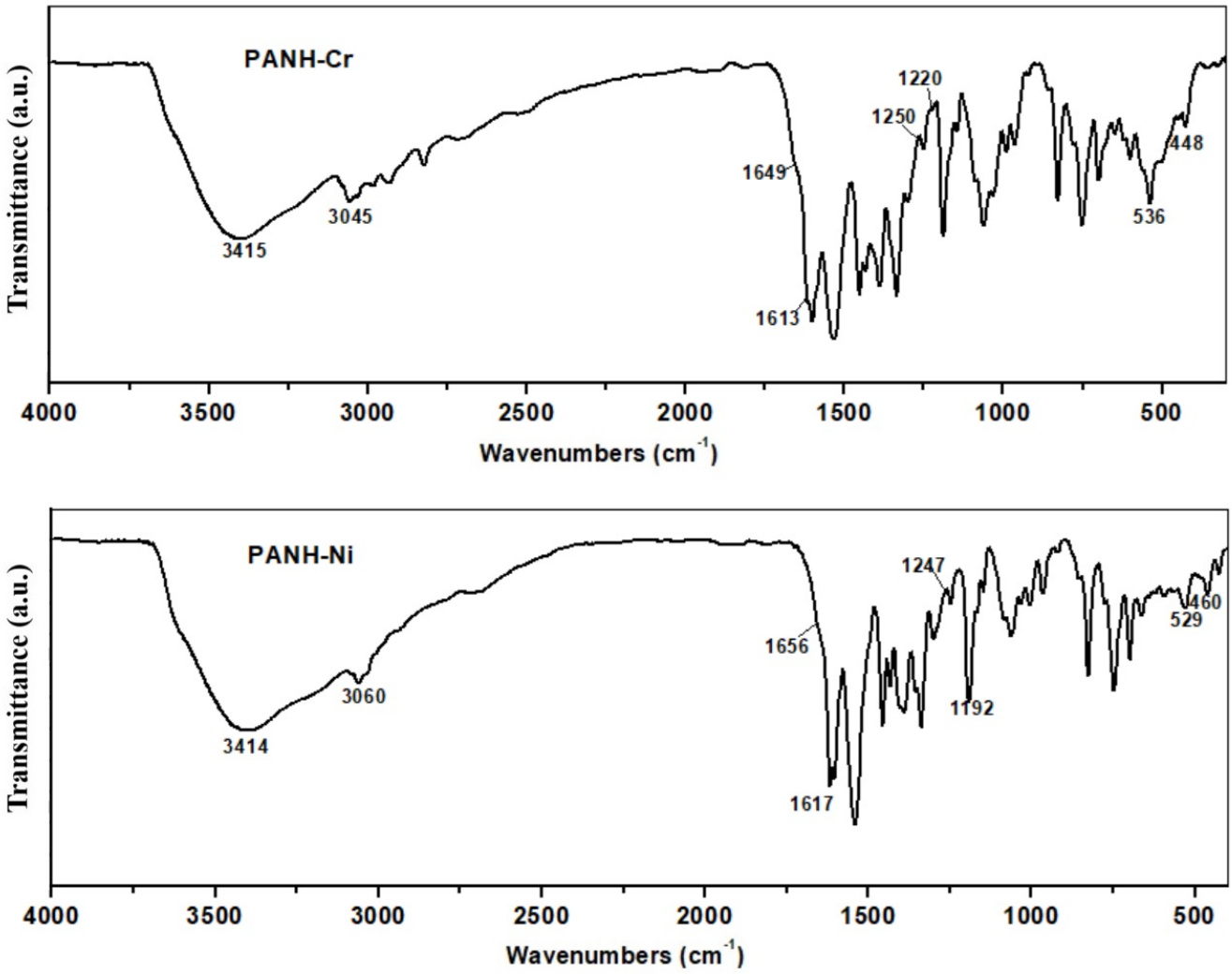

Fig. S5. IR spectra of **PANH-Cr** &**PANH-Ni** complexes

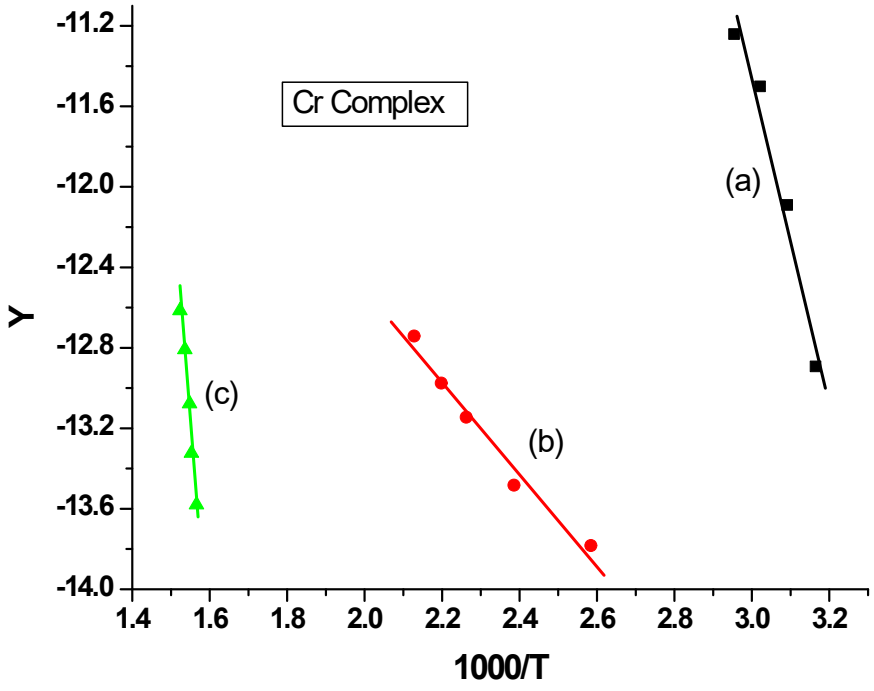

Fig. S6. Coats-Redfern plot for **PANH-Cr** complex.
a) first step b) second step c) third step
where, $Y= [-\ln(1- \alpha)] / T^2$ for $n = 1$

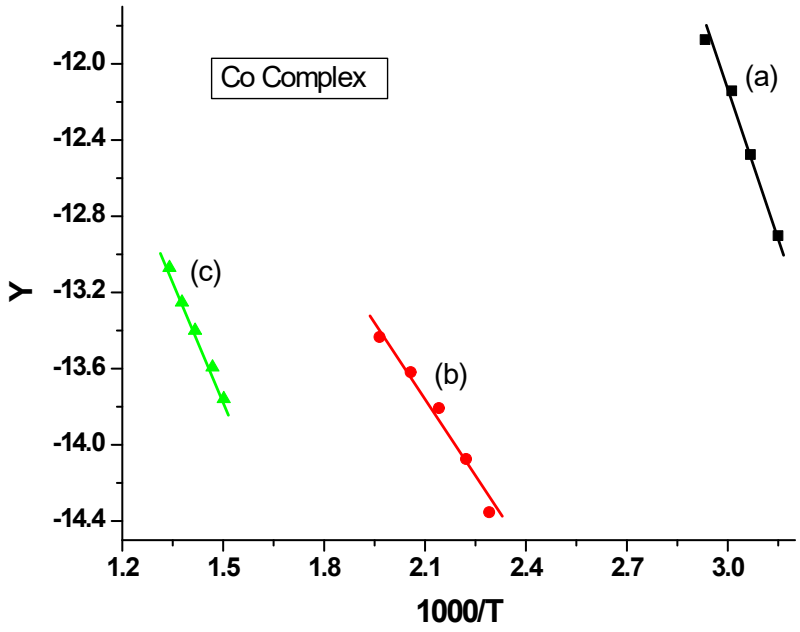

Fig. S7. Coats-Redfern plot for **PANH-Co** complex.
a) first step b) second step c) third step
where, $Y= [1-(1-\alpha)^{1-n}] / (1-n)\ T^2$ for $n \neq 1$ or $Y= [-\ln(1- \alpha)] / T^2$ for $n = 1$

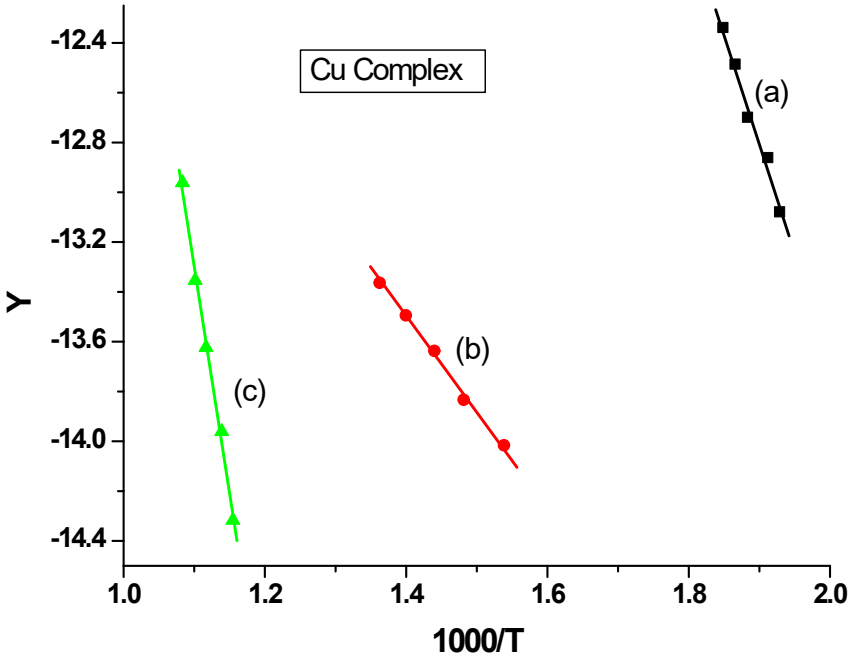

Fig. S8. Coats-Redfern plot for **PANH-Cu** complex.
a) first step b) second step c) third step
where, $Y= [1-(1-\alpha)^{1-n}] / (1-n)\ T^2$ for $n \neq 1$ or $Y= [-\ln(1-\alpha)] / T^2$ for $n = 1$

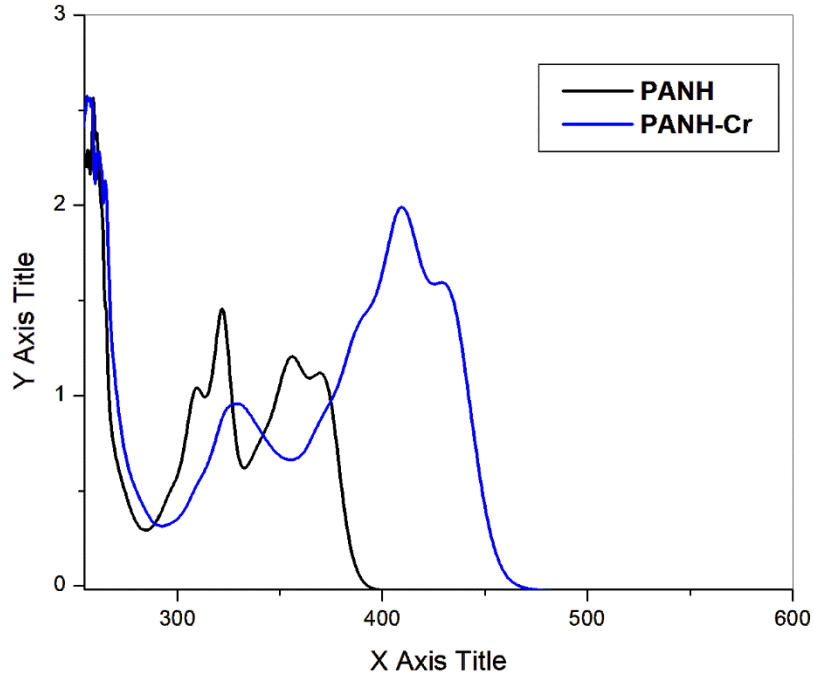

Fig. S9. UV-Vis spectra of PANH ligand and its Cr complex

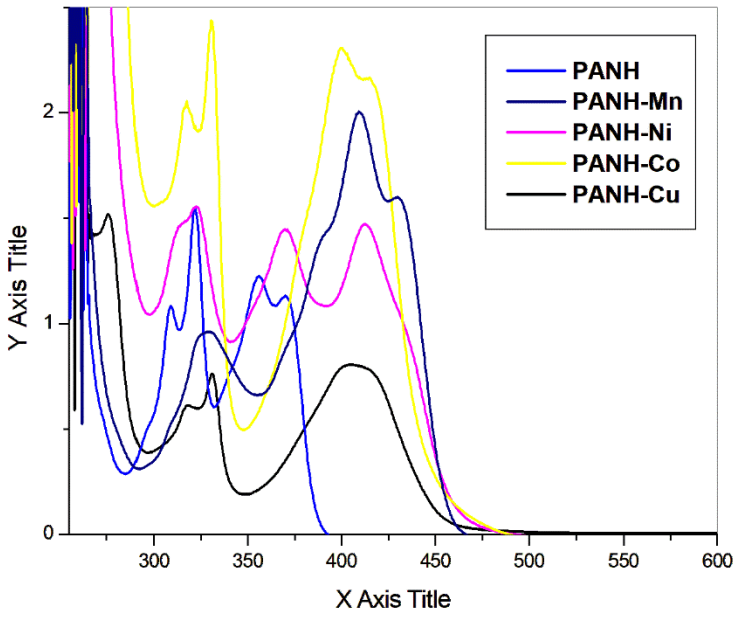

Fig. S10. UV-Vis spectra of PANH ligand and its Cr complex

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