Reviewer B:

1. **DFT optimization of Co(II) complexes should be done.**

The Co(II) was optimized and the geometric parameters were included. The optimized geometry of the Co(II) complex was included in the main text.

**2.**  **Page 4; sentence "B3LYP 6-31G(d,p) basis set '' is wrong, B3LYP is**

**functional and not basis set, so please correct into "B3LYP functional and**

**6-31G(d,p) basis set".**

The sentence was changed as suggested by the reviewer.

**3.** **The similar at page 7; sentence "B3LYP/ LANL2DZ function with**

**6-31G(d,p) basis set" should be corrected with "B3LYP functional together**

**with LANL2DZ and 6-31G(d,p) basis sets "**

The sentence has been corrected as per reviewers comment.

**4.** **Figures S1, and S3 are missing so please provide Figures for all spectra**

**(FT-IR, UV-Vis and NMR) in the Supplementary**.

The spectra were included in the supplementary. The figures S1 and S3 were also included.

**5.** **Table S2, please check transitions for Cu(II). The authors stated in the**

**text "The Cu(II) complex 2 showed a broad band around 850-950 nm …" and in**

**the Table S2 they assigned λmax = 584; please correct these values.**

The value in table has been changed as 850-950 nm.

**6. In the experimental part authors stated that "Electronic spectra of the**

**ligand and the complexes were recorded in DMSO" and then in Results section**

**they said "The UV-Vis spectra of the ligand and the metal complexes were**

**recorded in solid state " please correct the solvent.**

In the experimental part the correction was made as “Electronic spectra of the ligand and the complexes were recorded in solid state”.

**7.** **Page 9 "ev" should be "eV"**

As mentioned ev was changed as eV.

**8.** **Please check references, references 28 and 34 are the same.**

The reference 28 is a book whereas 34 is a journal. In reference 34 volume and page number was missing which have been included.

**9**. **Page 3, please give full name for "EDTA"**

EDTA was written as Ethylenediaminetetraacetic acid.