Synthesis of a new Acetate Bridged Cu(II) Building Block Generated 1D Polymer and Studies on Structural, Magnetic, Antibacterial and Anticancer Properties

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Electronic Supplementary Information (ESI)

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UV-vis spectral, FTIR and temperature dependent magnetization analysis of cluster **1**

Figures

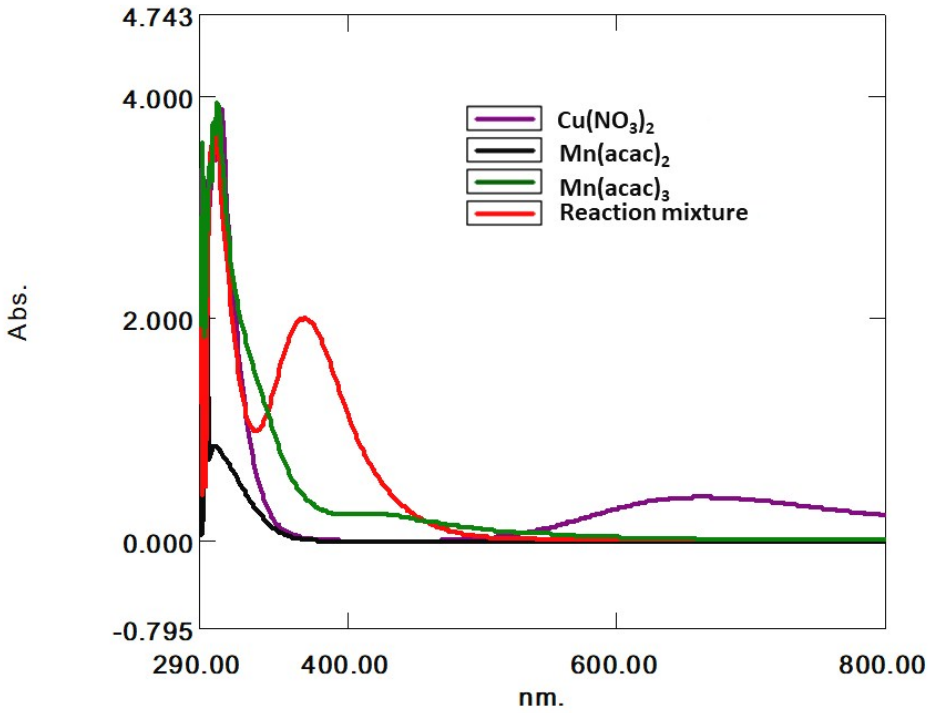

Fig. SI 1 (A): UV-vis spectra of (i) $Cu(NO_3)_2$, (ii) $Mn(acac)_2$, (iii) $Mn(acac)_3$ and (iv) Reaction mixture of complexation

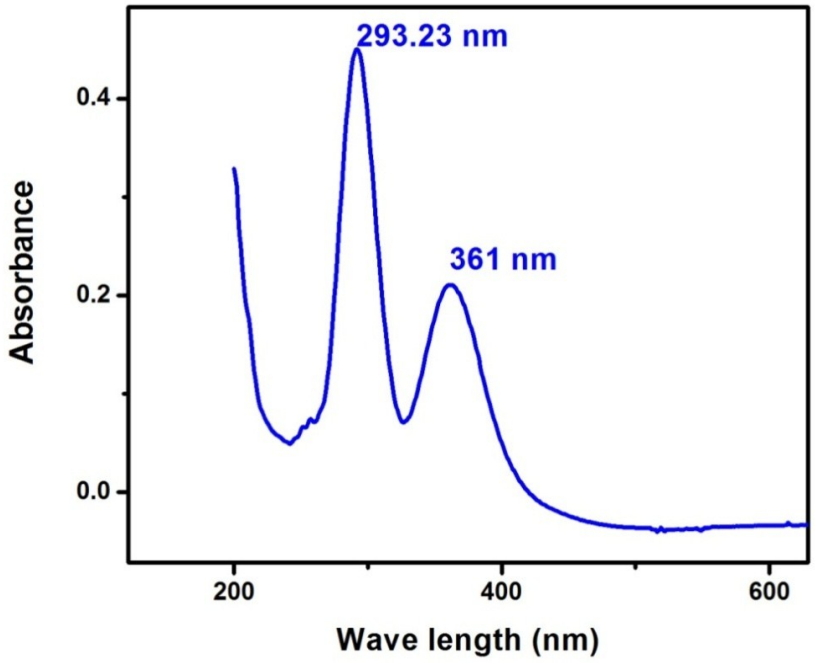

Fig. SI 1(B): UV-vis spectrum of complex **1** in methanol**.**

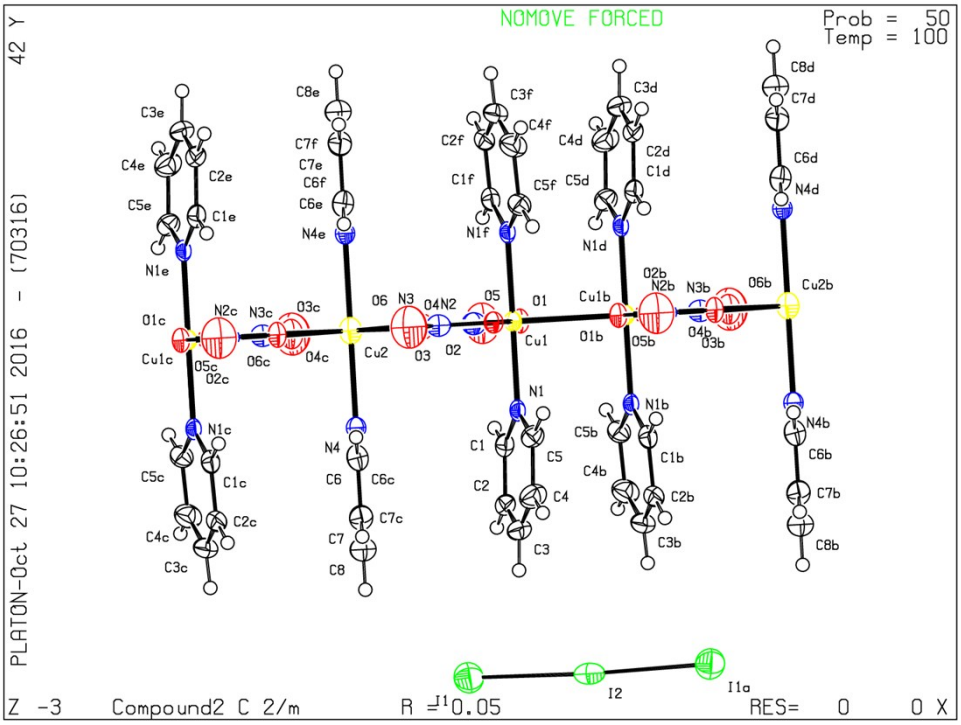

Fig. SI 2: Partially labeled ORTEP diagram of the 1D-polymeric cluster **1**. Thermal ellipsoids are drawn with 50 % probability.

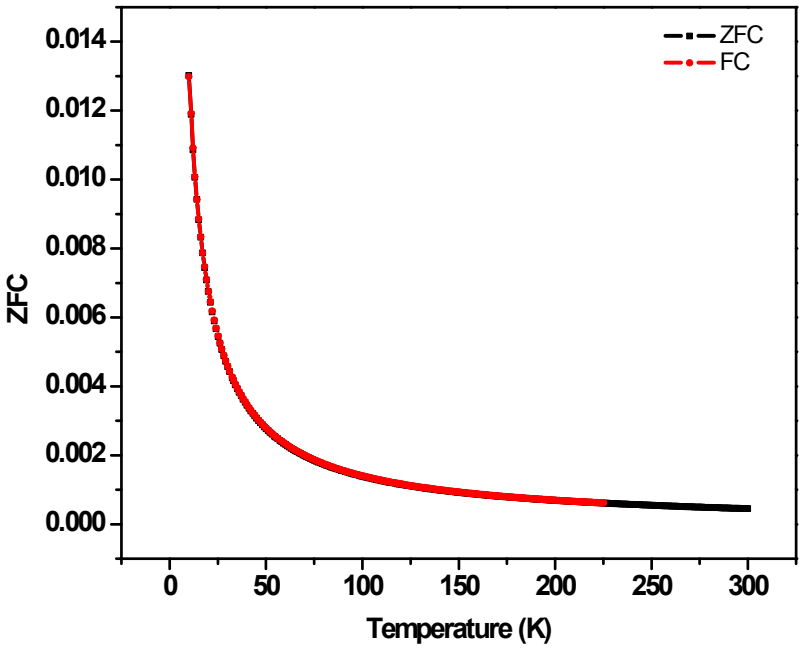

Fig. SI 3. Temperature dependent magnetization plots of complex **1** at 100 Oe.

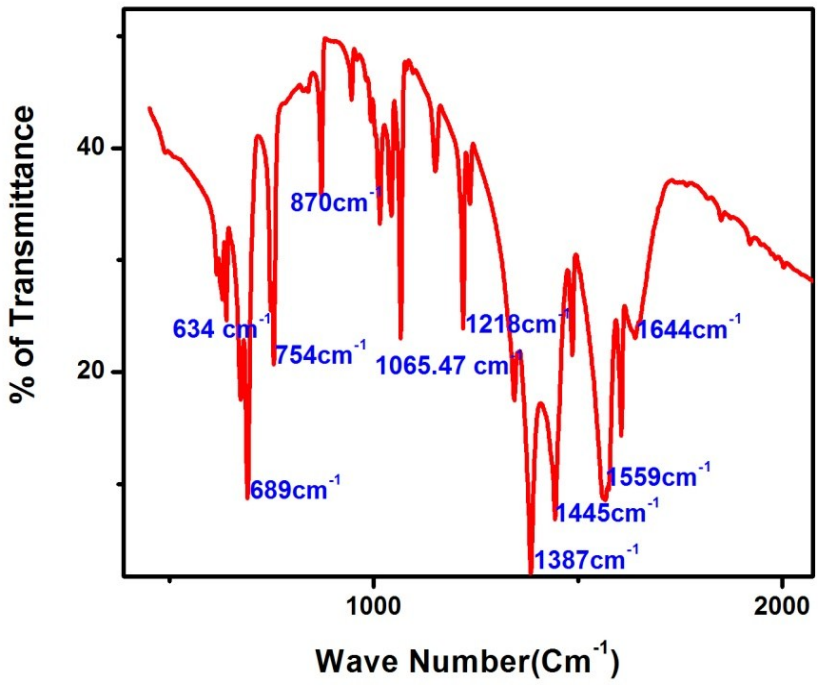

Fig. SI 4: FTIR spectrum of complex **1.**

Discussion

Existence of Mn^{3+} ions in the reaction mixture:

We have conducted a qualitative test for the detection of Mn^{2+} by using $NaBiO_3$ and HNO_3 (Ref. Book: Qualitative Inorganic Analysis by Vogel's) from the reaction mixture, but no pink colouration was observed. It clearly suggests that there is no existence of Mn^{2+} in the solution. It might be due to change of oxidation state of Mn from $Mn^{2+} \rightarrow Mn^{3+}$ in the presence of solid I_2. The formation of I_3^- in the solution can also be confirmed by the complexation as observed in the crystal structure. However in the reaction mixture the oxidation state of copper remained unchanged. Thus it is evident that Mn^{2+} ion participates in the one electron transfer process forming I_3^- with a subsequent formation of Mn^{3+} in solution.

$$Mn^{2+} + I_2 \rightarrow Mn^{3+} + I_3^-$$

We have also separately measured the

(i) UV-vis spectrum of $Mn(acac)_2$ which did not show any d-d transition band as Mn present in +2 state (Fig. SI 1 (A)).

(ii) UV-vis spectrum of $Cu(NO_3)_2$ which showed absorbance maxima at 662 nm indicating the presence of Cu in +2 state (Fig. SI 1 (A)).

(iii) UV-vis spectrum of $Mn(acac)_3$ where a weak absorption maxima appeared ~418 nm showing the presence of manganese in +3 state

(Fig. SI 1 (A)). [$Mn(acac)_3$ was prepared following a standard protocol; 1:2.5 ratio of $MnCl_2$ and CH_3COONa was dissolved in water and then added to acetylacetone and 2% $KMnO_4$ solution and heated at 60^oC for 10 minutes and cooled to give Shining black crystal of $Mn(acac)_3$].

(iv) In the UV-vis spectral measurement conducted from reaction mixture, two major peaks appeared at 291 and 365 nm (Shown in Fig. SI 1 (A)), seemingly due to complex formation. However, the absorption band with maximum near 365 nm is extremely broad in nature and thus we speculate that the small peak near 418nm, responsible for Mn^{3+} ions, might be hidden under the broad spectrum.

UV-VIS Spectra analysis:

The electronic spectra of the complex was recorded in methanol solution. The complex exhibits two absorption bands at 293 nm and 361 nm (**Fig. SI 1(B)**). The absorption band at 293 nm could be due to ligand centred transition and the absorption band at 361 nm could be due to the d-d transitions for the Cu(II) ions present in the complex **1** in octahedral enviornment.

Temperature dependent magnetization: Fig. SI 3 shows temperature dependent magnetization studies (from 2 to 300 K) carried out on complex **1** at 100 Oe in zero field cooled (ZFC) and field cooled (FC) condition. Nature of

temperature dependent magnetization plots suggest weak ferromagnetic moments in Cu complex.

FTIR analysis:

The infra-red spectrum of the complex **1** is represented in **Fig. SI 4**. The sharp band at 689 cm^{-1} can be assigned to the ν (Cu-O) vibrational mode. The small shoulder at 634 cm^{-1} can be assigned as Cu-N stretching frequency. The absorption bands from 1644-1445 cm^{-1} can be assigned as the C=C and C=N stretching vibrational mode which confirms the co-ordination of the ligand with the metal atoms.