Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Figures and Tables

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Figures

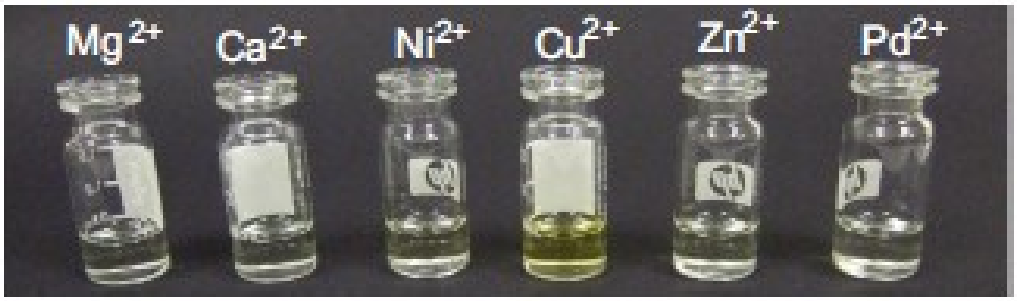

Fig. S1 . Color changes observed on addition of 3-HNHBH ligand to $Mg(OAc)_2$, $Ca(OAc)_2$, $Ni(OAc)_2$, $Cu(OAc)_2$, $Zn(OAc)_2$ and $Pd(OAc)_2$ solutions

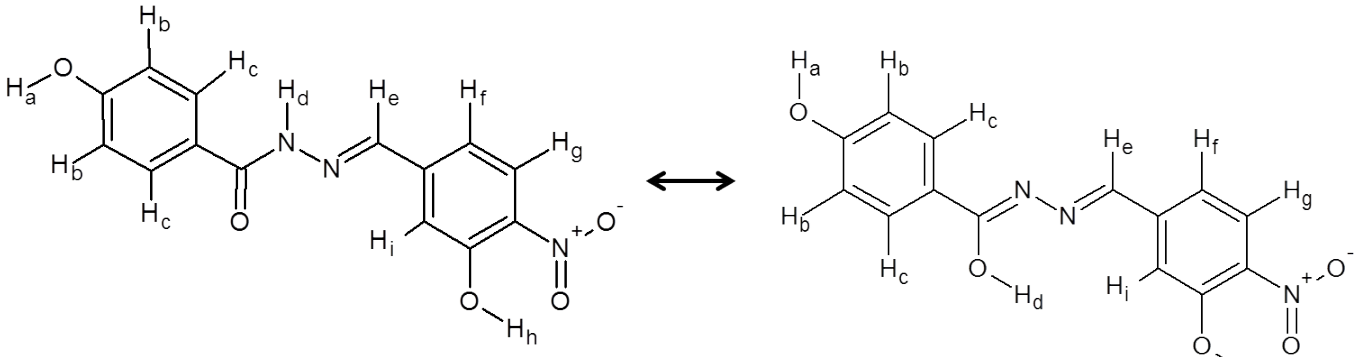

Fig. S2 Hydrogen assignment in keto (a) and enol (b) forms of 3-HNHBH ligand

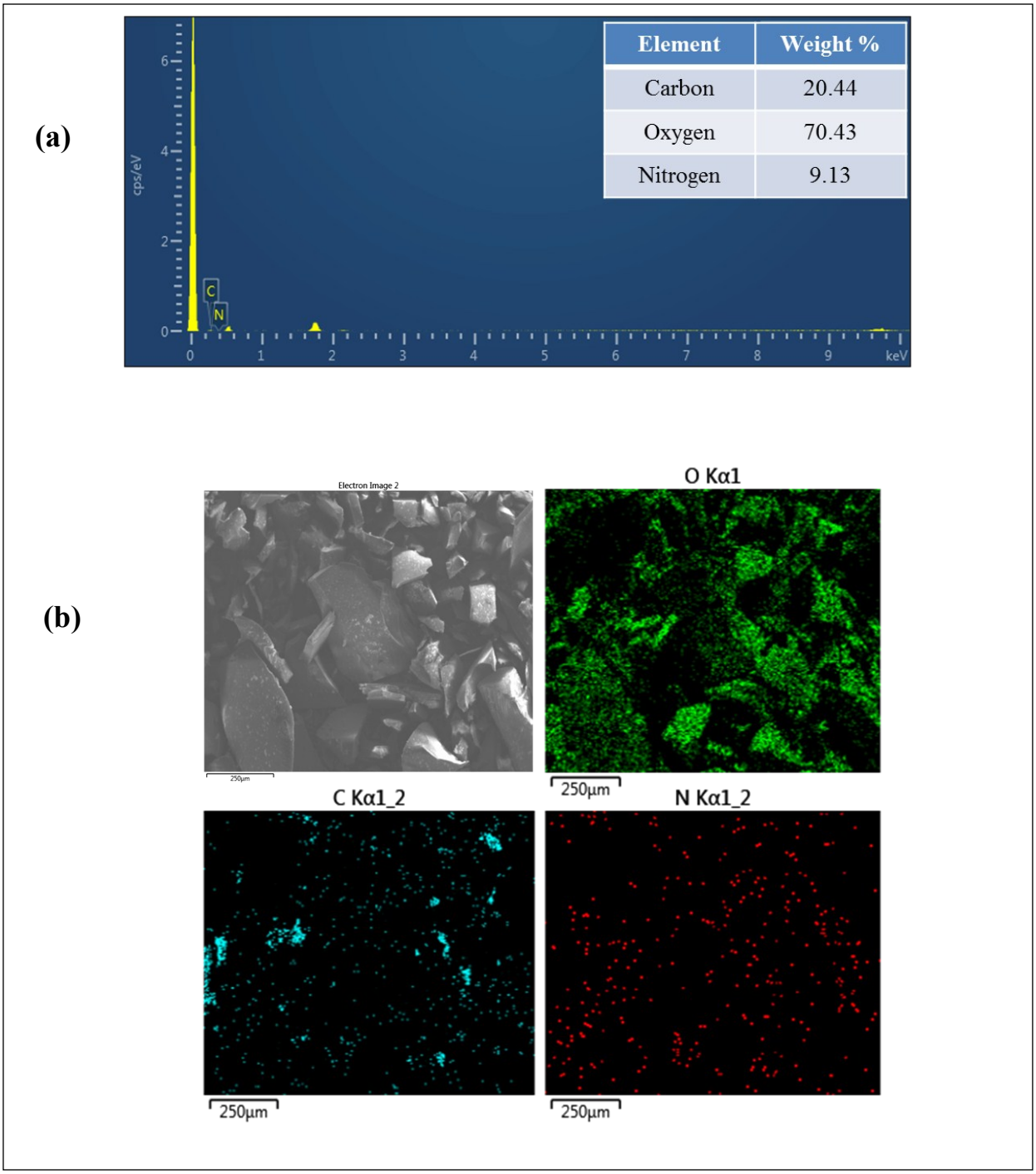

Fig. S3 (a) EDX spectrum, and (b) EDX elemental mapping of 3-HNHBH ligand

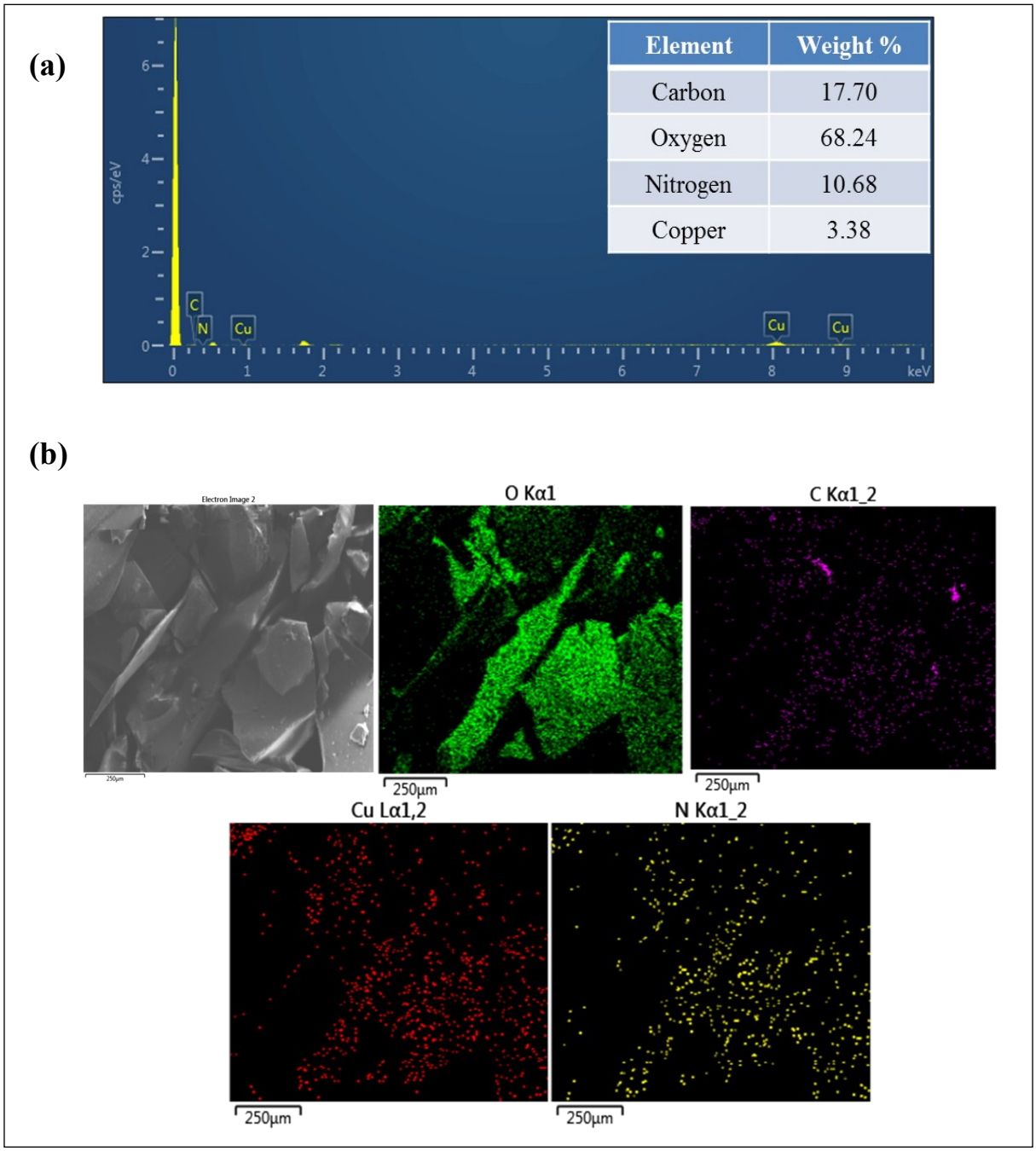

Fig. S4 (a) EDX spectrum and (b) EDX elemental mapping of 3-HNHBH after complexation with Cu(II) ion.

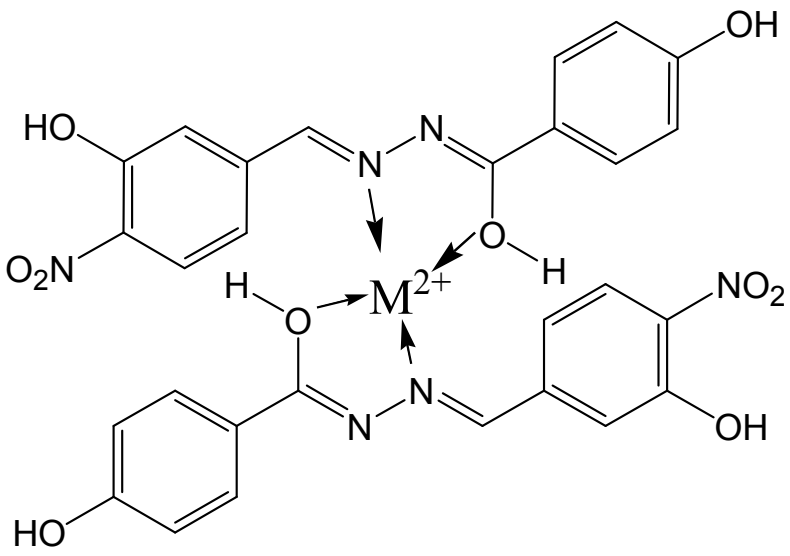

Fig. S5 Proposed mode of complexation of 3-HNHBH ligand and metal ions

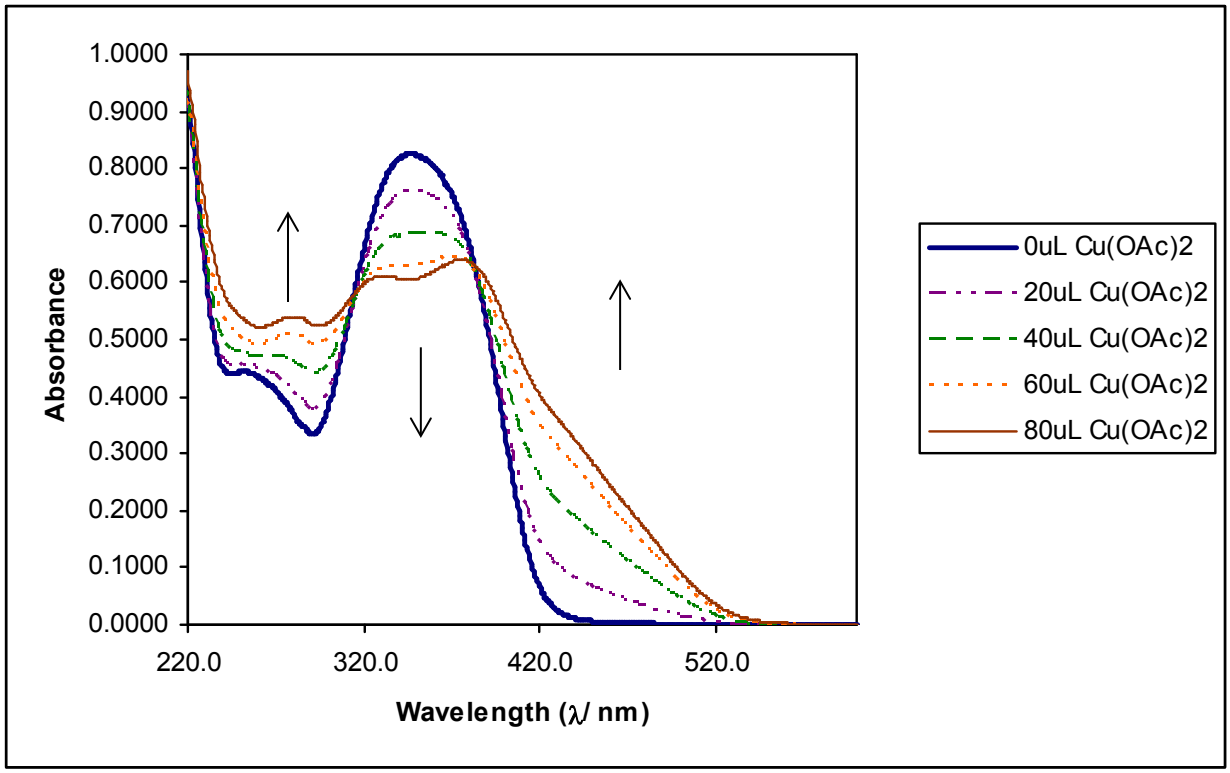

Fig. S6 Absorbance vs wavelength (λ/ nm) of ligand/THF with $Cu(OAc)_2$/ACN. Some spectra omitted for clarity

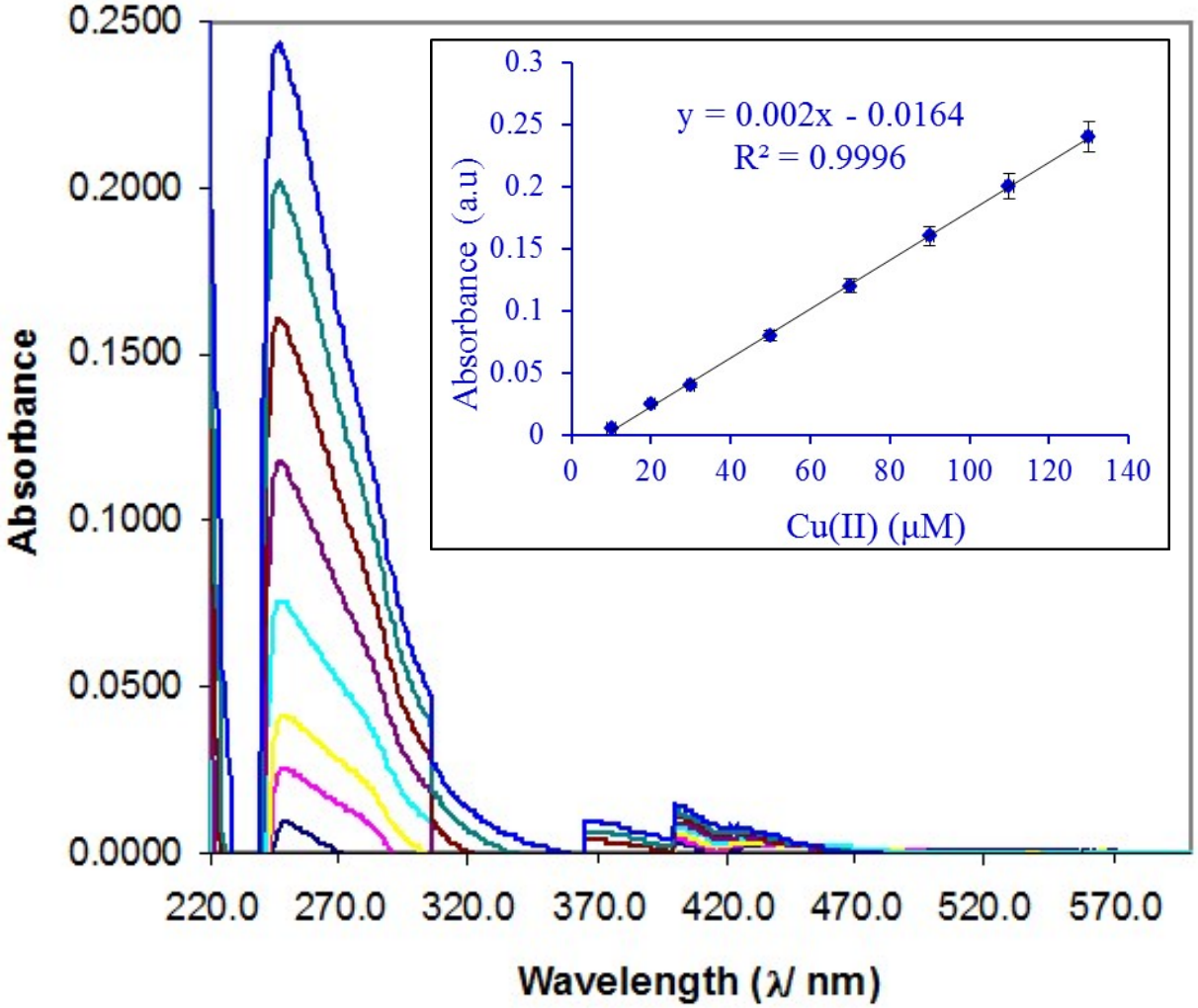

Fig. S7 Absorbance vs wavelength (λ/ nm) of ligand/THF with increasing concentrations of Cu(II) ions. Some spectra omitted for clarity. Inset: Calibration plot of absorbance vs concentration of Cu(II) ions

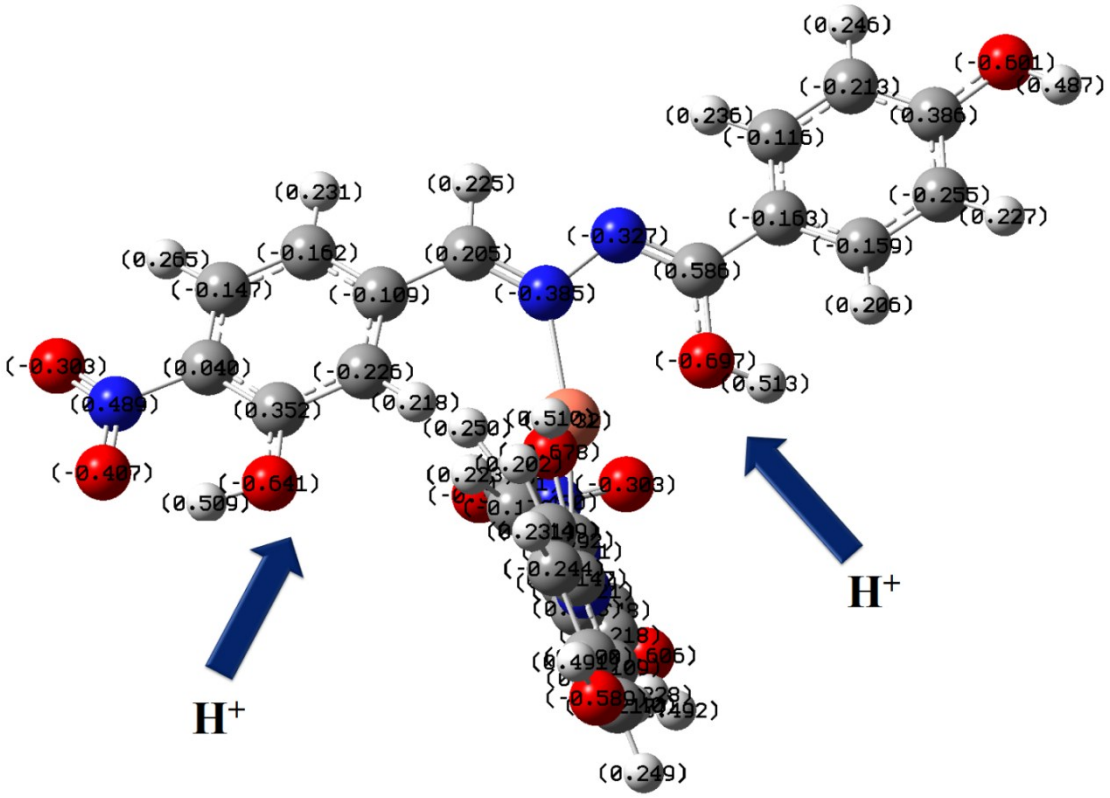

Fig. S8 Mulliken atomic charges distribution of 3-HNHBH ligand complex with Cu(II) ion as calculated at the B3LYP/6-311+G* level. The arrows indicate potential sites for possible proton attack

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Tables

Table S1 ^{1}H NMR assignment of 3-HNHBH ligand before and after complexation

Proton	Ligand/DMSO-d_6		Ligand-Cu/DMSO-d_6	
	Chemical shift δ/ ppm	**Splitting pattern**	**Chemical shift δ/ ppm**	**Splitting pattern**
H_a	11.17	Singlet	11.72	Singlet
H_b	7.81	Doublet	9.40	Singlet
H_c	6.87	Doublet	7.77	Singlet
H_d	10.18	Singlet	12.64	Singlet
H_e	8.38	Singlet	8.22	Singlet
H_f	7.28	Doublet	6.84	Singlet
H_g	7.96	Doublet	6.84	Singlet
H_h	11.86	Singlet	11.72	Singlet
H_i	7.49	Singlet	6.84	Singlet

Table S2 Color of ligand/THF solutions on addition of metal salts in THF or ACN

Solvent		
Solute	**THF**	**ACN**
$Zn(OAc)_2$	**Solution remains pale greenish-yellow**	**Solution remains pale greenish-yellow**
$Cu(OAc)_2$	**Solution turns slightly darker shade of greenish-yellow**	**Solution turns yellow (distinct, intense colour change)**
$Ni(acac)_2$	**Solution turns (pale) orange-yellow**	**Solution turns pale orangey-yellow**

Table S3 Color change on addition of EDTA and HCl to 3-HNHBH ligand and metal salts in mixed aqueous solutions

Concentration of EDTA / M	**2×10^{-2}**		**2×10^{-4}**		**2×10^{-2}**	
Vol. of EDTA or HCl added	**+1µL EDTA**	**+1µL HCl**	**+10µL EDTA**	**+10µL HCl**	**+1µL EDTA**	**+1µL HCl**
Solvent composition Solute [Initial solution colour]	**25% THF mixed aqueous solution**		**50% THF mixed aqueous solution**		**75% THF mixed aqueous solution**	
$Ni(acac)_2$	**Yellow**	**Solution turns colourless**	**Bright yellow**	**Solution turns colourless**	**Green-yellow**	**Solution turns colourless**
$Cu(OAc)_2$	**Yellow**	**Solution turns colourless**	**Bright yellow**	**Solution turns colourless**	**Green-yellow**	**Solution turns colourless**
$Zn(OAc)_2$	**Yellow**	**Solution turns colourless**	**Bright yellow**	**Solution turns colourless**	**Green-yellow**	**Solution turns colourless**