SUPPORTING INFORMATION

Tridentate chelating ligand based fluorescentZn(II) coordination compounds for highly selective detection of picric acid

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PXRD of complexes 1 and 2

The X-ray powder diffraction (PXRD) patterns of bulk samplesand simulated ones obtained from the single crystal XRD data of complexes **1** and **2**are compared in Fig. 1S: the result shows that simulated PXRD pattern indicates consistency with that of the correspondent bulk sample of **1** and **2**.

Electronic absorption spectra of complexes

The absorption spectrum of **HL** shown in Fig.13S exhibits two broad bands at 350 and 450nm with its maximum centered at 400nm ($\varepsilon \sim 1.43 \times 10^4$ $Lmole^{-1}$ cm^{-1})and 414 nm ($\varepsilon \sim 1.44 \times 10^4$ L $mole^{-1}$ cm^{-1}); that ofcomplex **1** at 387nm ($\varepsilon \sim 0.8 \times 10^4$ $Lmole^{-1}$ cm^{-1}) and complex **2** at 388 nm ($\varepsilon \sim 1.21 \times 10^4$ $Lmole^{-1}$ cm^{-1}).The absorption properties of both the complexes in presence of different nitroaromatic compounds were investigated by adding equal amount of analytes. Upon the addition of an identical amount of different nitroaromatic compounds, a different degree of hyperchromic shift was observed for both complexes (Fig. 9S).

ESI mass spectrometry

The ESI mass spectrum of **1** (Fig.14S) recorded in methanol shows a peak at m/z = 785.17, corresponding to $[C_{38}H_{26}Zn_2N_{10}O_2]^+$ (calc. m/z = 785.46). On the other hand, the spectrum of **2** (Fig.15S) shows a peak at m/z = 737.26, corresponding to $[C_{34}H_{26}Zn_2N_{10}O_2]^+$ (calc. m/z = 737.42). These results evidence that in solution the polymeric complex**1**underwentfragmentation to dinuclearspecies, whilecomplex **2** in methanolmaintains the structure detected in solid state.

Table 1S. π···π Stacking interactions distances (Å) and angles (°) for compound **2**.[a]

Cg(I)	Cg(J)	Symmetry Cg(j)	Cg(I)-Cg(J)	α	β	γ	slippage
py-N2	py-N8	1-x,1-y,1-z	4.2561(16)	19.85(13)	25.8	45.2	1.849
py-N4	py-N6	2-x,1-y,1-z	4.0398(15)	17.39(13)	40.8	23.7	2.642
C24/C29	py-N6	-1+x, -1+y, z	4.2390(17)	15.48(14)	41.2	28.9	2.795

[a]Cg(*I*)-Cg(*J*): distance between ring centroids; *α*: dihedral angle between planes Cg(*I*) and Cg(*J*); *β*: angle Cg(*I*) → Cg(*J*) vector and normal to plane I; *γ*: angle Cg(*I*) → Cg(*J*) vector and normal to plane *J*; slippage: distance between Cg(*I*) and perpendicular projection of Cg(*J*) on ring *I*.

Table 2S. Fluorescence life time (ns) of complexes **1** and **2**, recorded in different conditions.

	Fluorescence life time
Complex **1**	0.66
Complex **2**	0.79
Complex **1**+ PA	0.63
Complex **2**+ PA	0.78

Table 3S. Comparison of picric acid sensing ability of complexes **1** and **2** with respect to otherZn(II) complexes.

Complex	**LOD (M)**	**K_{sv} (M^{-1})**	**Reference**
1	1.30603×10^{-6}	2.8×10^5	this work
2	2.9819×10^{-6}	2.3×10^5	this work
$Zn_4(DMF)(urotropine)_2(NDC)_4$	7.1×10^{-6}	10.83×10^4	16a
$[CH_3)_2NH_2]_3[Zn_4Na(BPTC)_3].4H_2O.2DMF$	5×10^{-6}	3.2×10^4	16b
$[Zn_2(NH_2BDC)_2(dpNDI)]_n$	1.31×10^{-6}	NA	16c
$[Zn_2LCl_2(H_2O)]$	3.986×10^{-9}	8.063×10^4	17c

$[Zn_2L(SCN)_2(H_2O)]\cdot H_2O$	3.974×10^{-9}	7.987×10^{4}	17c
$[Zn_2L(N_3)(CH_3CO_2)]$	3.914×10^{-9}	8.51×10^{4}	17c

(16a) S. Mukherjee,A.V. Desai, B. Manna, A.I. Inamdar,S.K.Ghosh, *Cryst.Growth Des.* 2015, 15, 4627-4634. NDC= 2,6-naphtalenedicarboxylic.

(16b)E.L. Zhou, P. Huang, C. Qin, K. Z. Shao, Z. Su, *J. Mater. Chem. A* 2015, 3, 7224-7228.BPTC = biphenyl-tetracarboxylic acid.

(16c) S.S. Dhankhar, N. Sharma, S. Kumar,T.J.D. Kumar, C.M. Nagaraja, *Chem. Eur. J.* 2017, **23**, 16204-16212. NH_2BDC = 2-aminoterephthalic acid, dpNDI = *N*,*N*′-di(4-pyridyl)-1,4,5,8-naphthalenediimide.

(17c) A. Das, S. Jana, A. Ghosh, *Cryst. Growth Des.*2018, 18, 2335–2348. L = *N,N*′-dimethyl-*N,N*′-bis(2-hydroxy-3-methoxy-5-methylbenzyl)ethylenediamine.

Table 4S. IR bands (cm^{-1}) of complexes **1-2**.

Selected bond	HL	complex **1**	complex **2**
ν (C_{sp2}-H)	3056 (w)	2921 (w)	3068 (vw)
ν C≡N)	-	2323, 2264, 2185 (s)	-
ν (N≡N)	-	-	2091, 2062 (s)
ν (C=N)	1624(s)	1622 (s)	1628 (s)
ν (ArC=C)	1543 (m)	1540 (m)	1540 (m)

m = medium, s = strong, w = weak, vw = very weak

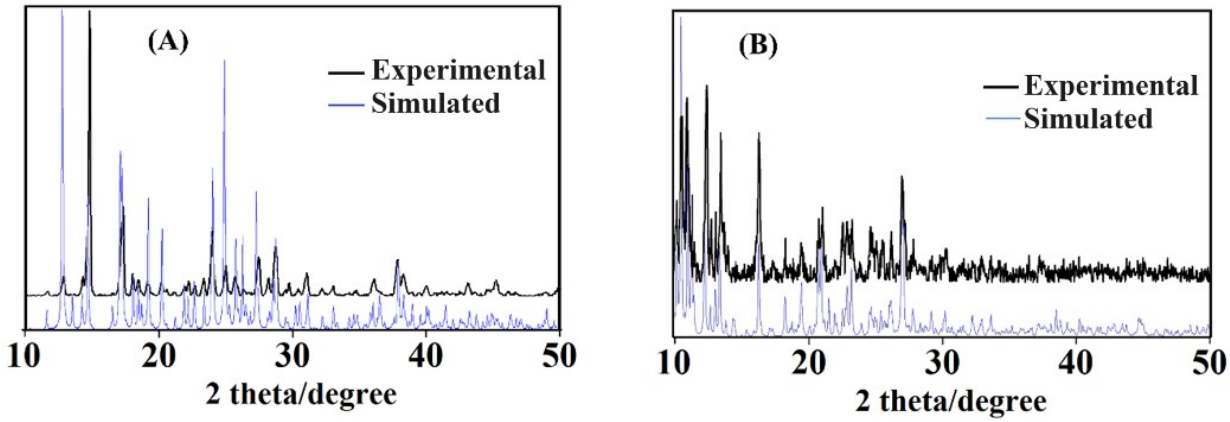

Fig.1S. Experimental and simulated X-ray diffraction patterns of complexes**1**(A)and **2** (B).

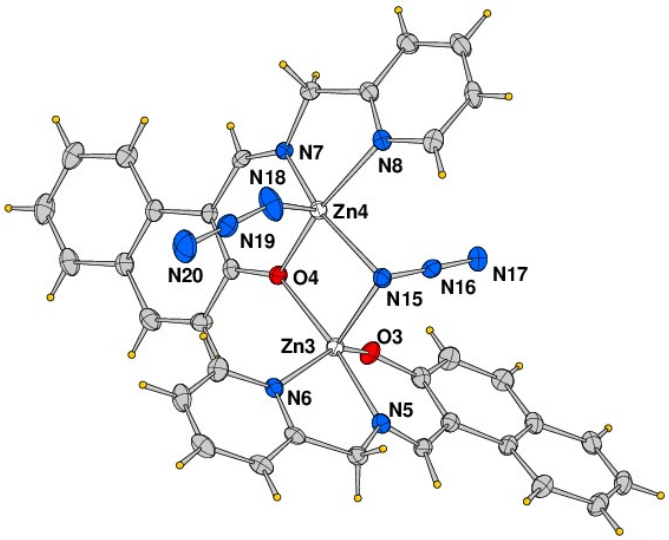

Fig.2S. Ortep view (ellipsoid probability at 50%) of complex B of compound 2.

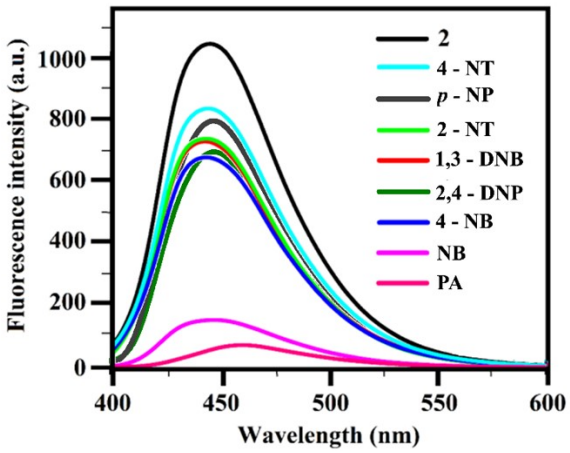

Fig.3S. Change of emission intensity of complex **1** (3 ml 2.16×10^{-7} M ≡ 6.48×10^{-10} moles) upon the addition of differentnitroaromaticcompounds (100 µL, 6.2×10^{-4} M ≡ 6.2×10^{-8} moles).

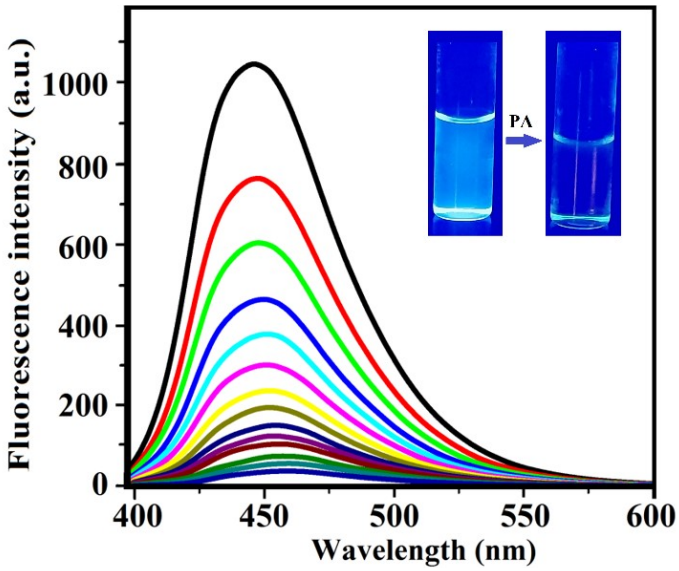

Fig.4S. Luminescence quenching of complex **2** by gradual addition of 4×10^{-4} M PA (20 µL-260 µL).(Inset: visual colour change of the complex solutions (under UV light, 366 nm) upon addition of PA.

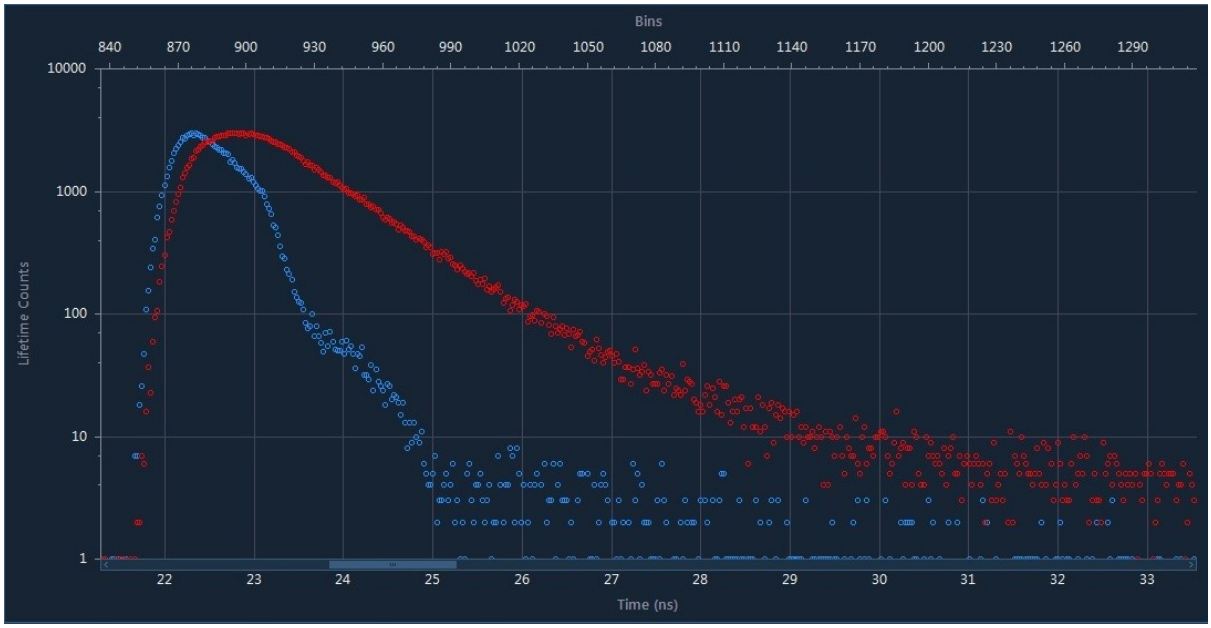

Fig.5S. Fluorescence lifetime decay profile of complex **1**.

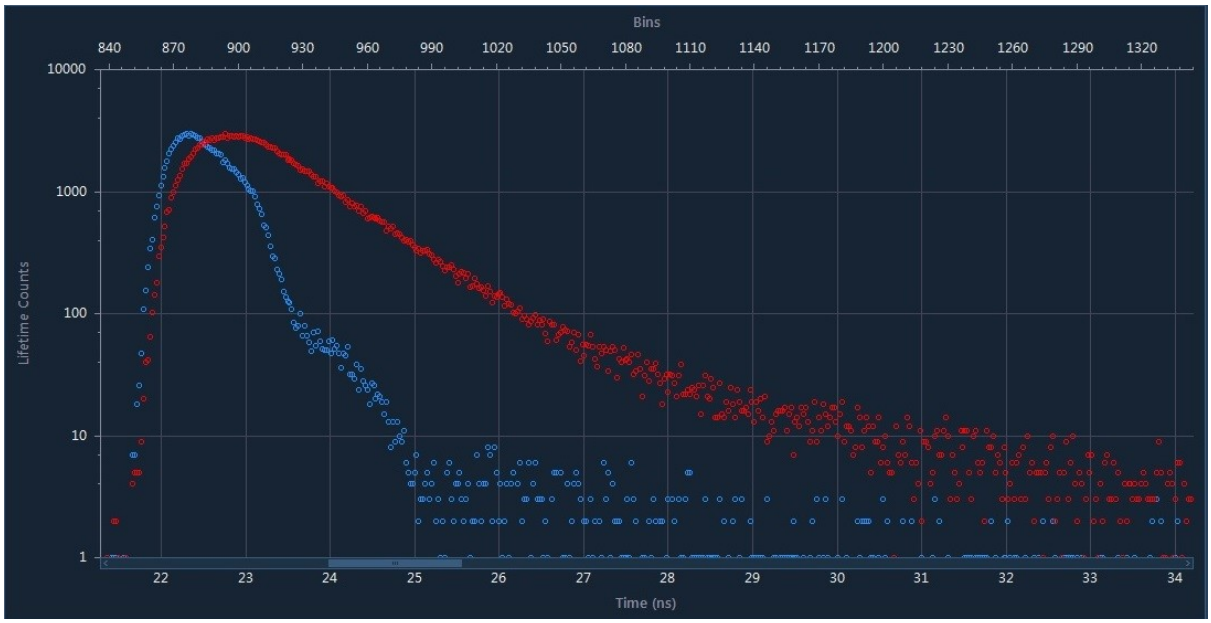

Fig.6S. Fluorescence lifetime decay profile of complex **2**.

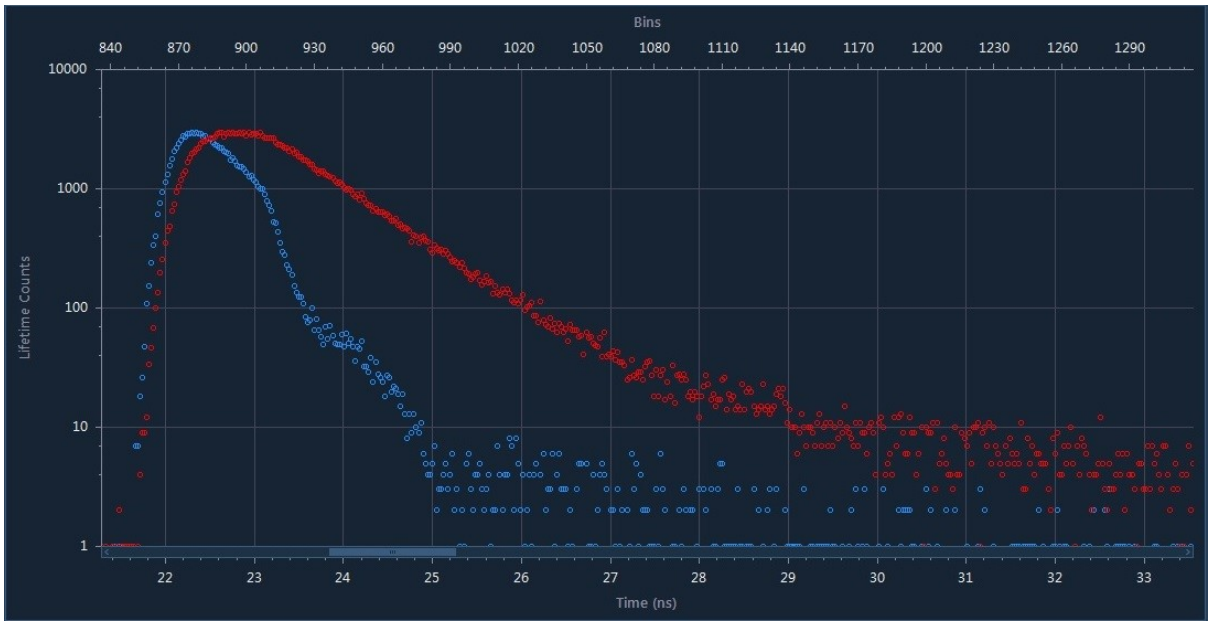

Fig.7S. Fluorescence lifetime decay profile of complex **1** after addition of PA.

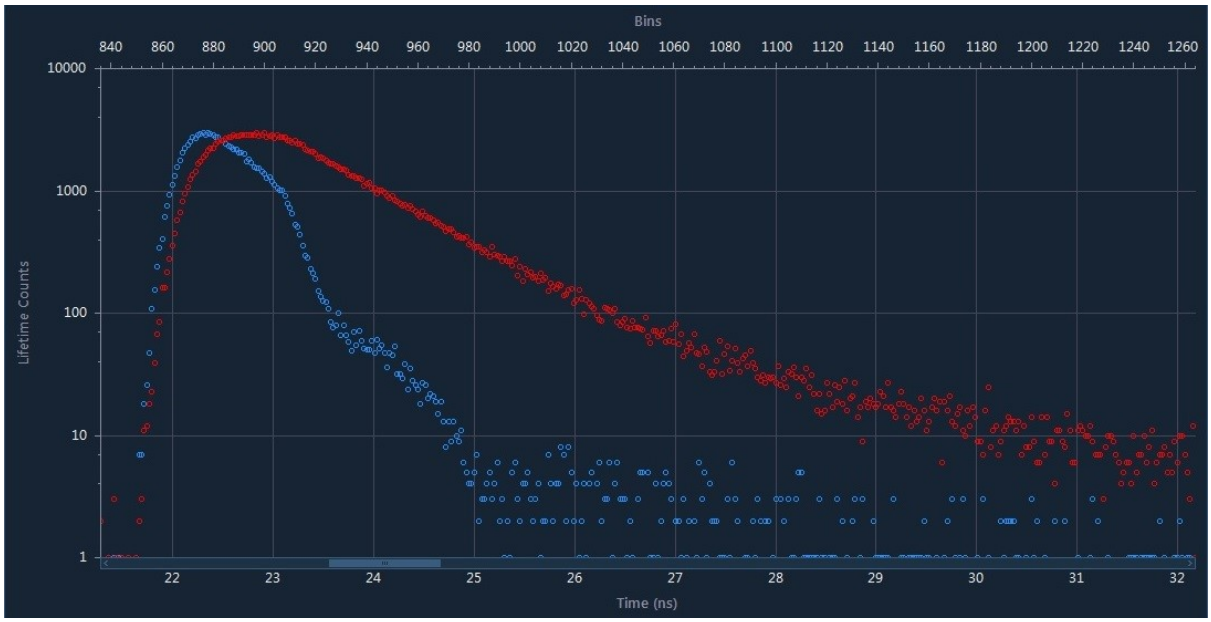

Fig.8S. Fluorescence lifetime decay profile of complex **2** after addition of PA.

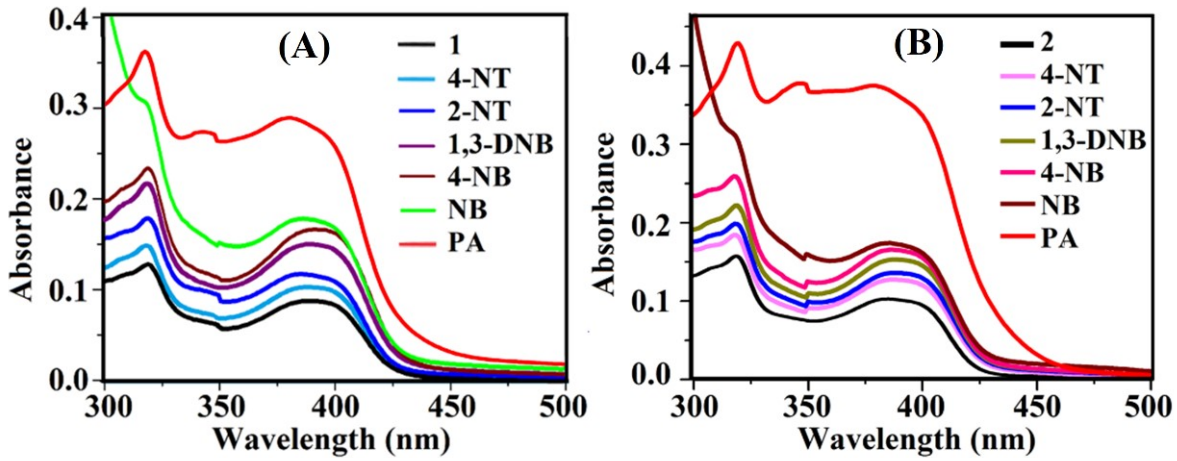

Fig.9S. Electronic spectra of complexes **1** (A) and **2** (B) in presence of different nitroaromatic compounds.

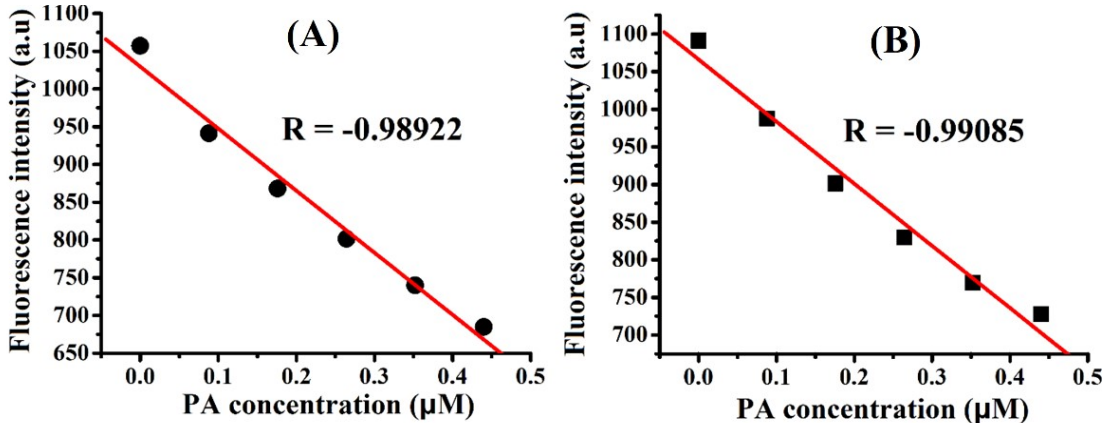

Fig.10S. Plot of fluorescence intensity of complexes *vs* concentration of PA [(A) for **1**; (B) for **2**].

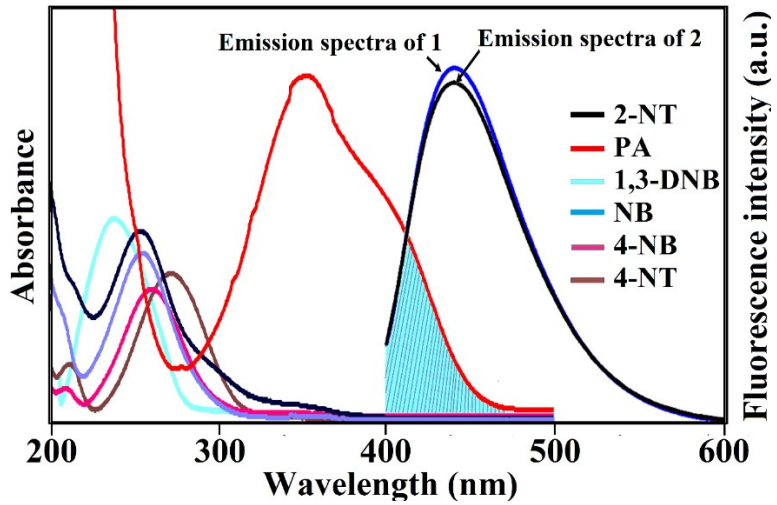

Fig.11S. Spectral overlap of the absorption spectra of analytes (including PA), and the emission spectra of complexes **1-2**.

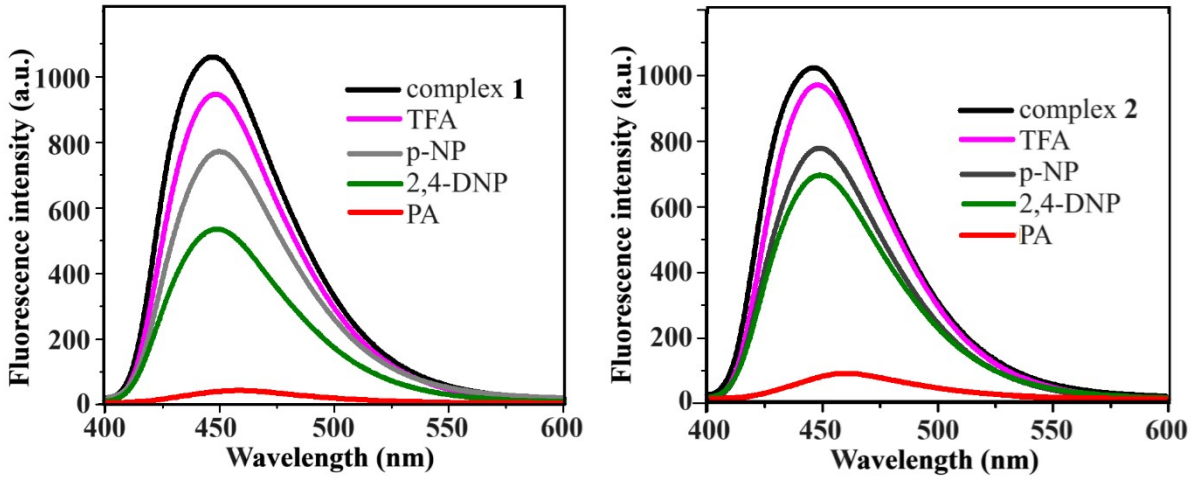

Fig.12S. Change of emission intensity of complexes **1** and **2** (50µL, 1.3×10^{-5} M ≡ 6.5×10^{-10} mole)upon the addition of TFA (trifluoroacetic acid), *p*-NP (*p*-nitrophenol), 2,4-DNP (2,4-dinitrophenol), PA (picric acid) analytes (100µL, 6.2×10^{-4} M ≡ 6.2×10^{-8} mole).

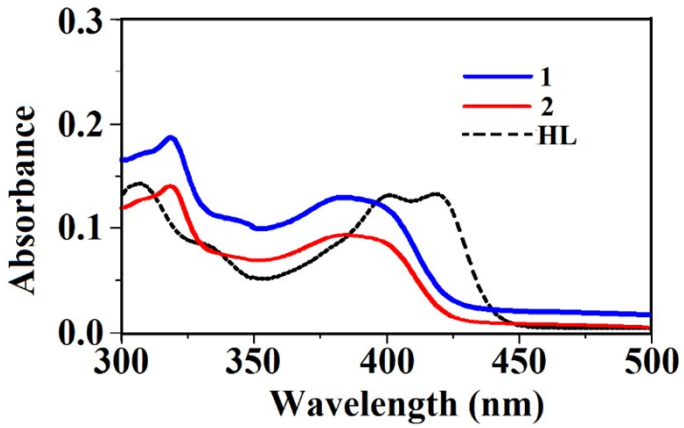

Fig.13S. Absorption spectra of **HL**, complexes **1** and **2** in methanol.

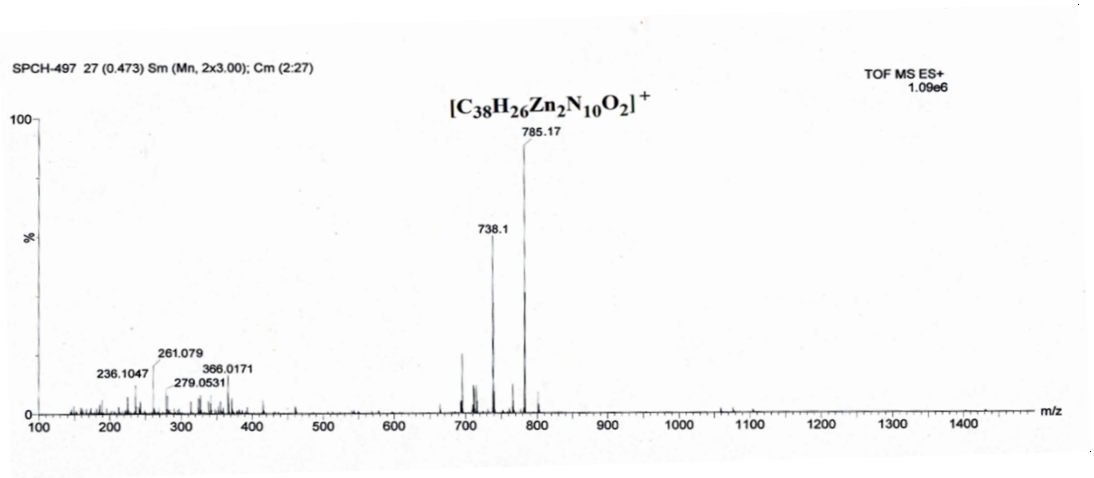

Fig.14S.ESI mass spectra of complex **1.**

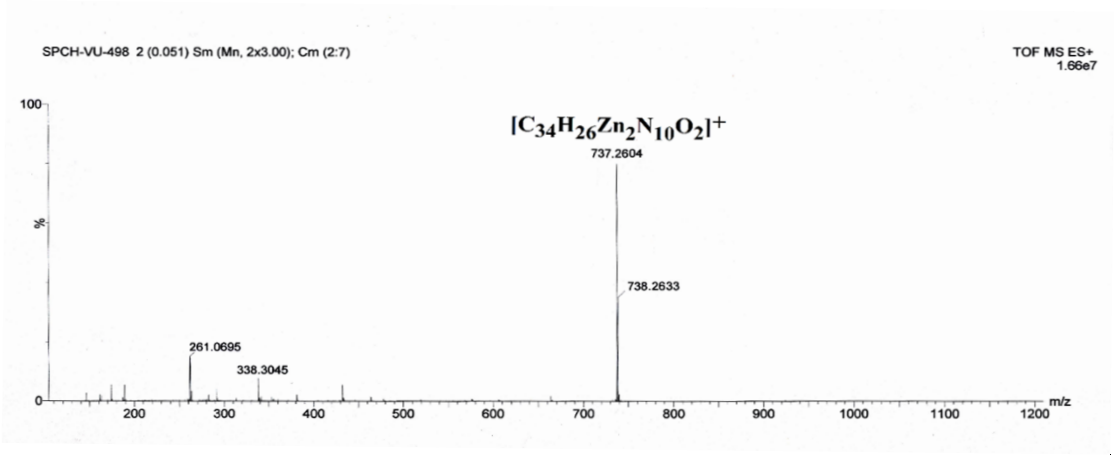

Fig. 15S. ESI mass spectra of complex **2**.

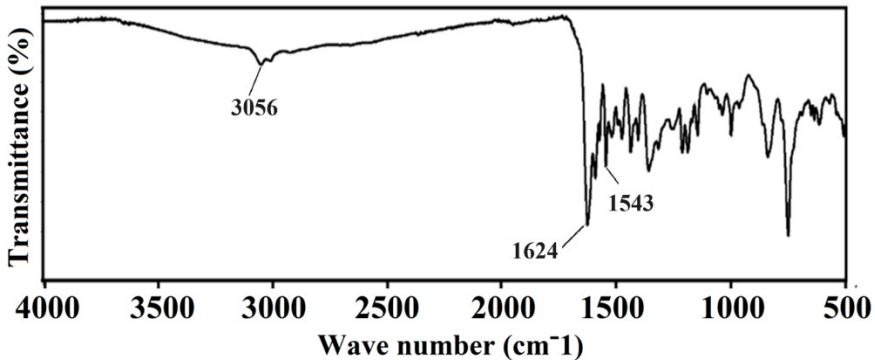

Fig.16S. FT-IR spectrum of free ligand (**HL**).

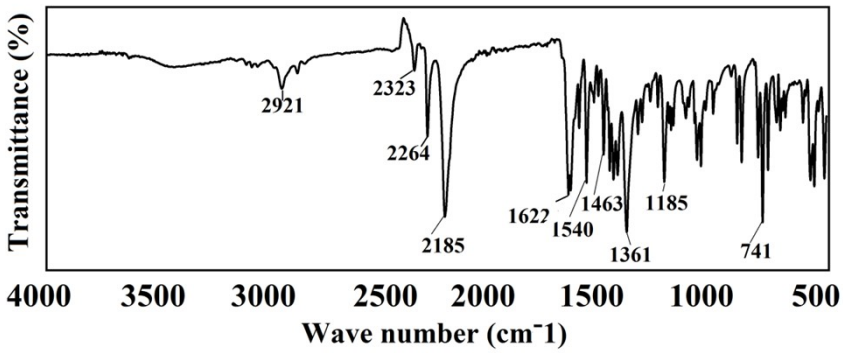

Fig.17S. FT-IR spectrum of complex **1**.

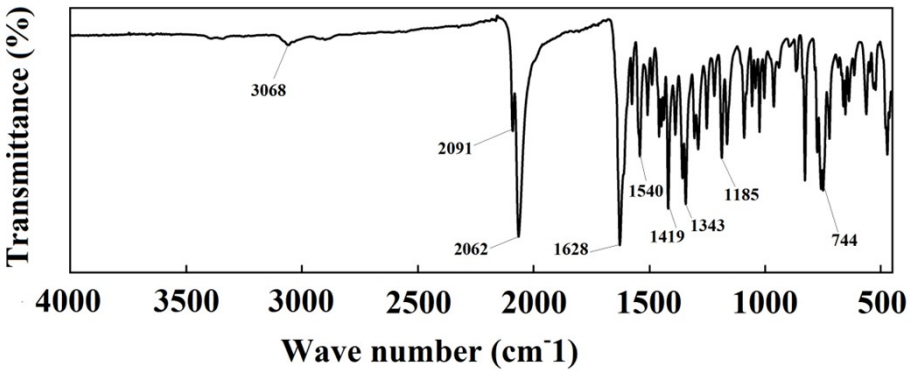

Fig.18S. FT-IR spectrum of complex **2**.

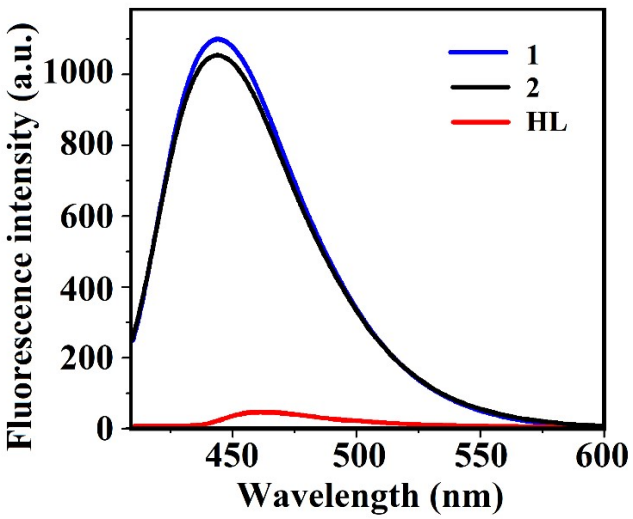

Fig.19S. Emission spectra of **HL** and of complexes **1** and **2** in methanol.

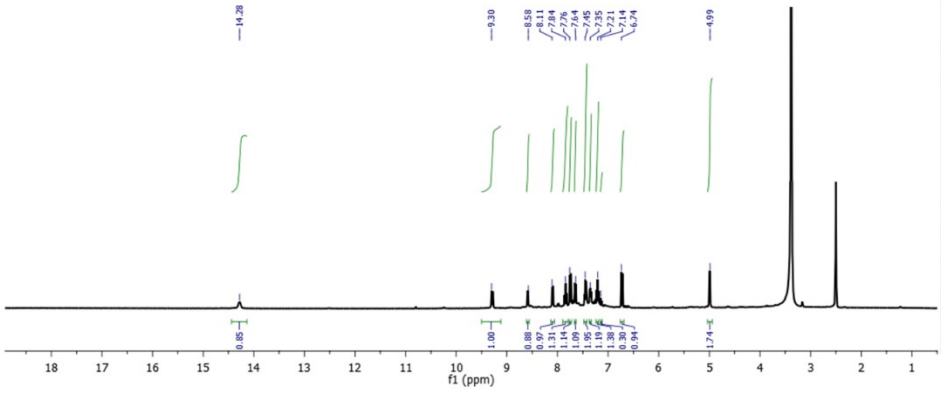

Fig.20S. ^{1}H-NMR spectrum of ligand in d_6-DMSO solvent

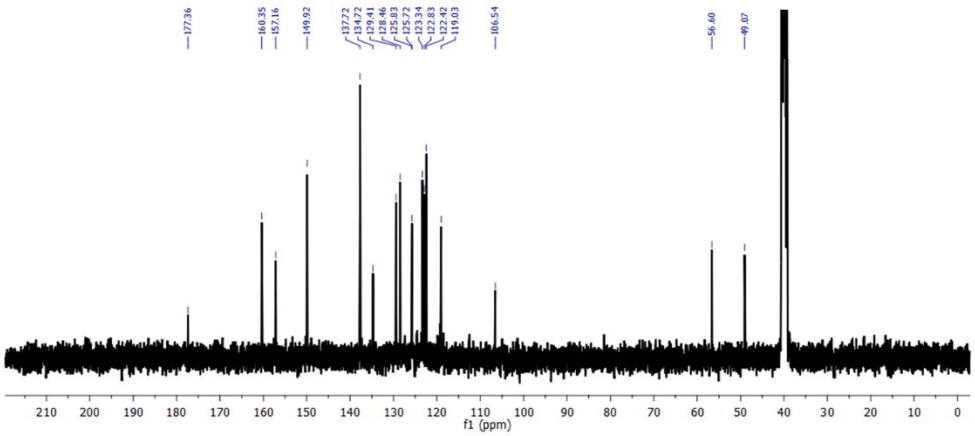

Fig.21S. ^{13}C-NMR spectrum of ligand in d_6-DMSO solvent

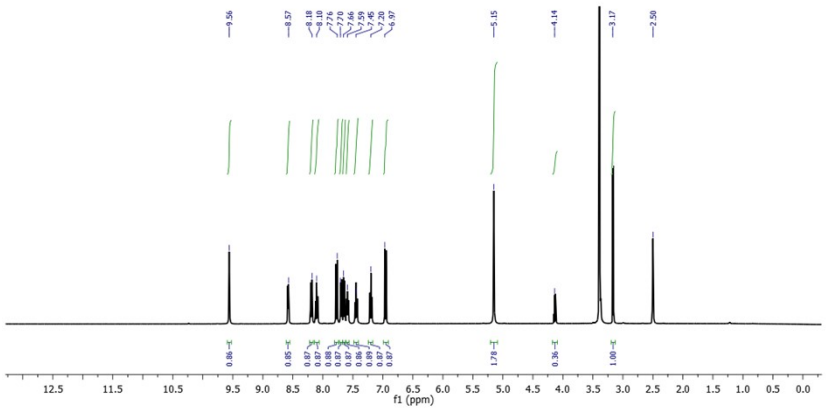

Fig.22S. ^{1}H-NMR spectrum of complex **1** in d_6-DMSO solvent.

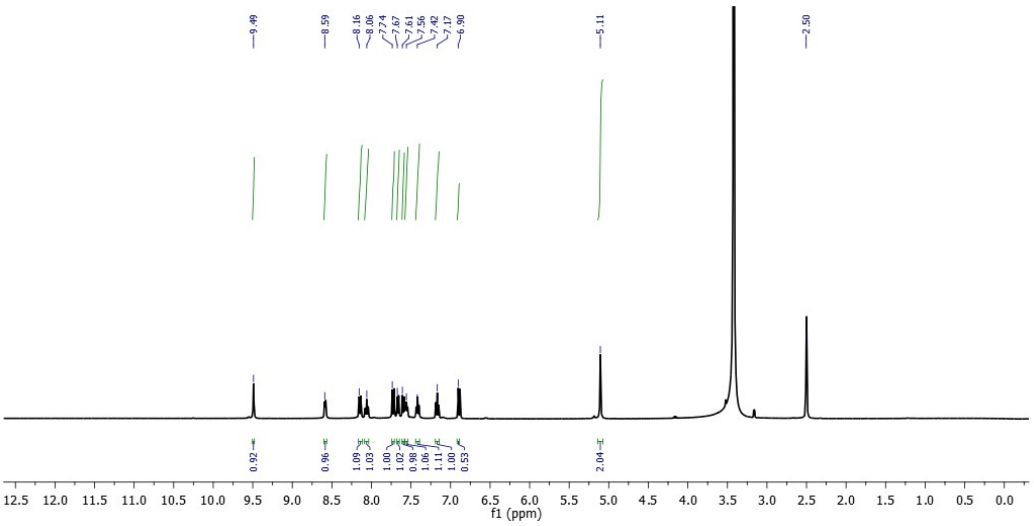

Fig.23S.[1]H-NMR spectrum of complex **2** in d_6-DMSO solvent

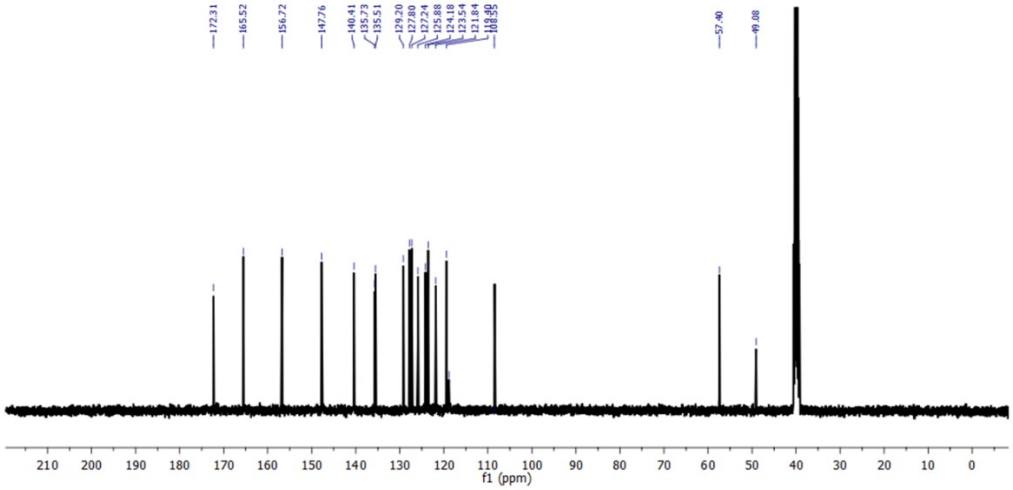

Fig.24S.[13]C-NMR spectrum of complex **1** in d_6-DMSO solvent

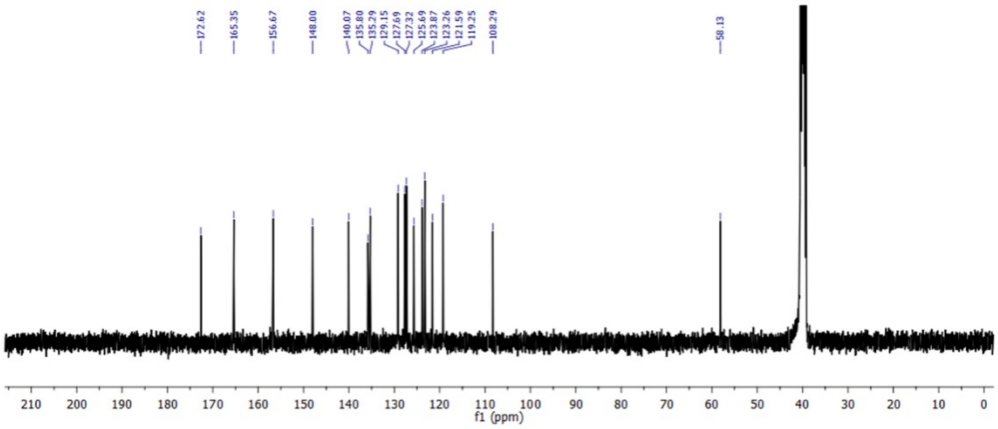

Fig.25S. [13]C-NMR spectra of complex **2** in d_6-DMSO solvent