Supporting Information

Solid-State Fluorescence Sensing of Amine Vapours by an Anthracene based Zn(II) Complex, its Phosphatase Activity and Theoretical Calculations

Alakananda Mahapatra[a], *Piyali Adak*,[a] *Shyamal Kumar Chattapadhay*[a]*

[a]Department of Chemistry, Indian Institute of Engineering Science and Technology, Howrah-711103, W.B. India

*Corresponding Author, Email: shch20@hotmail.com

List of Contents

Materials and instrumental details:

Materials:

We have purchased 9-anthracenealdehyde(Sigma-Aldrich 97%), N,N-dimethylethylenediamine(Spectrochem,98%), Sodium borohydride(Spectrochem 96%), Zinc Chloride(Sigma-Aldrich 98%), 4-nitrophenylphosphate disodium salt hexahydrate (Spectrochem 99%) and all amines of reagent grade were used as such. Also DMF, HPLC Water, Acetone, DMSO, Methanol, DCM and absolute ethanol were purchased from Spectrochem Pvt. Ltd.

Instruments:

We have used FTIR Spectrometer (Agilent Technologies FTIR-630) for FTIR study, (spectrometer region 4000 cm^{-1} to 650 cm^{-1}), BRUKER NMR (400 MHz) for NMR studies(2.50 ppm ^1H NMR chemical shifts for DMSO) ,D_2O was used as a reference solvent residue signal. For regular UV-vis spectral analysis, we have used a JASCO UV-V530 spectrophotometer. A Photon Technology International (PTI) spectrophotometer (Horiba, Delta diode) and a multifunctional time-correlated single-photon counting (TCSPC) fluorescence spectrophotometer (Model 1057, Fluorlog, Horiba Scientific Tech., USA) were used to collect the fluorescence data.

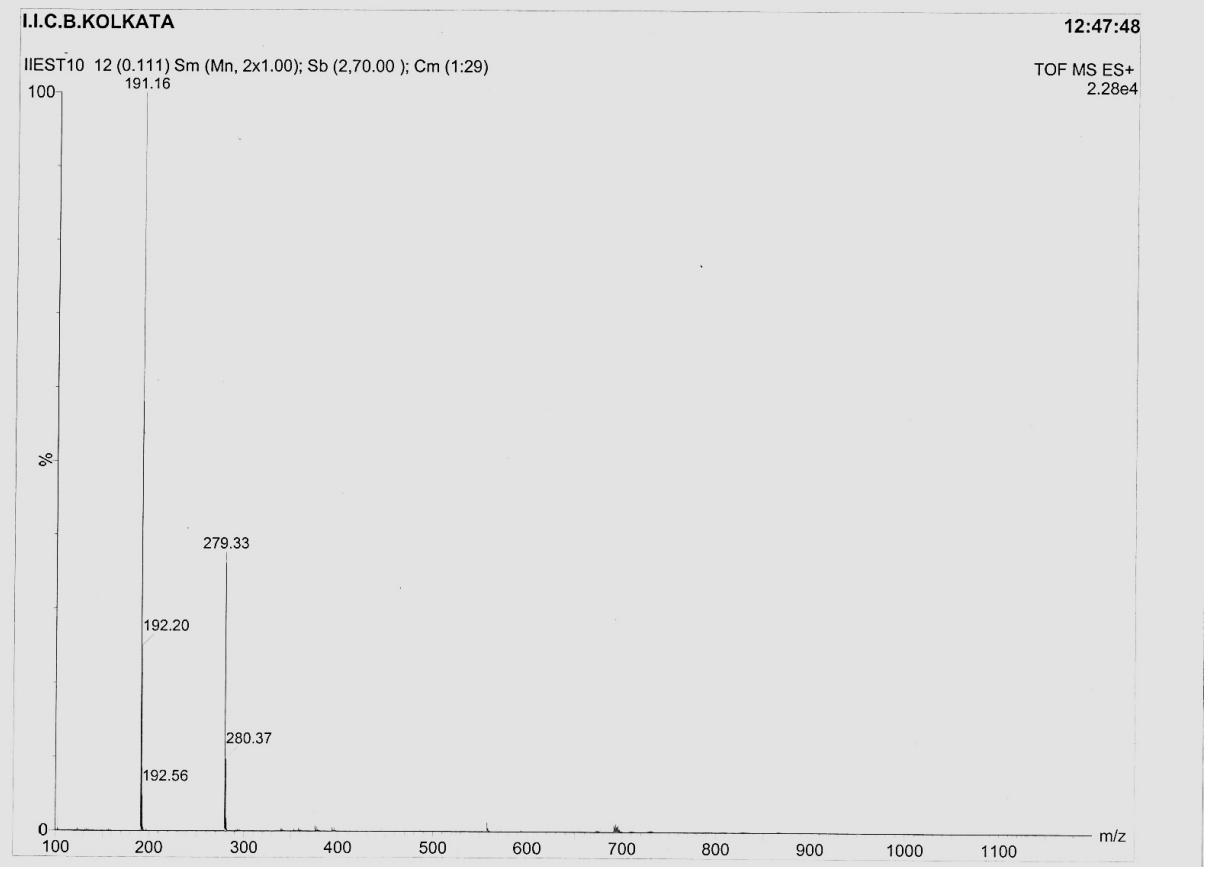

Figure S1. ESI-MS spectrum of ligand.

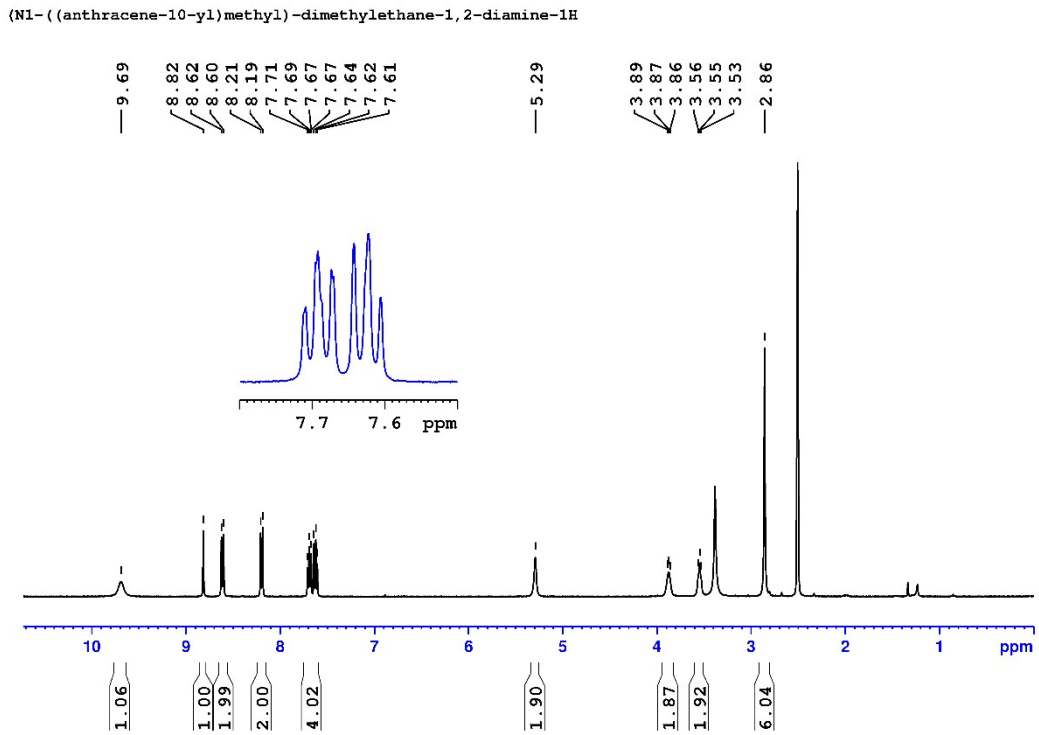

Figure S2. NMR spectrum of ligand

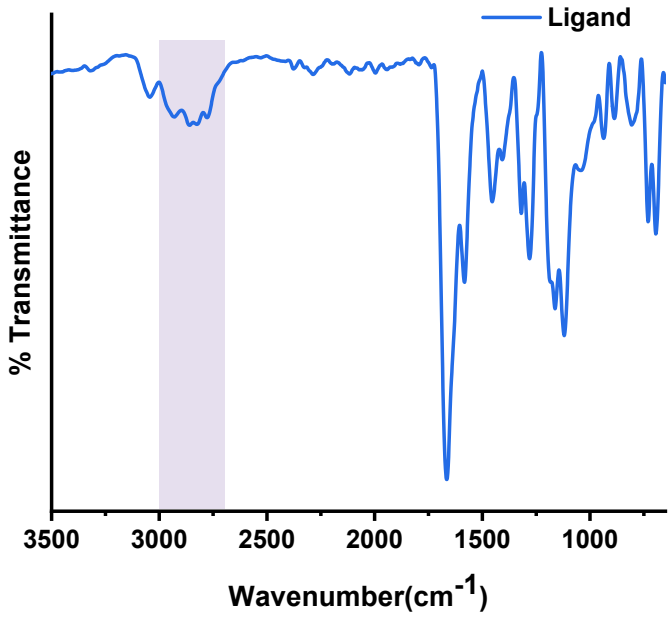

Figure S3. FTIR spectrum of ligand.

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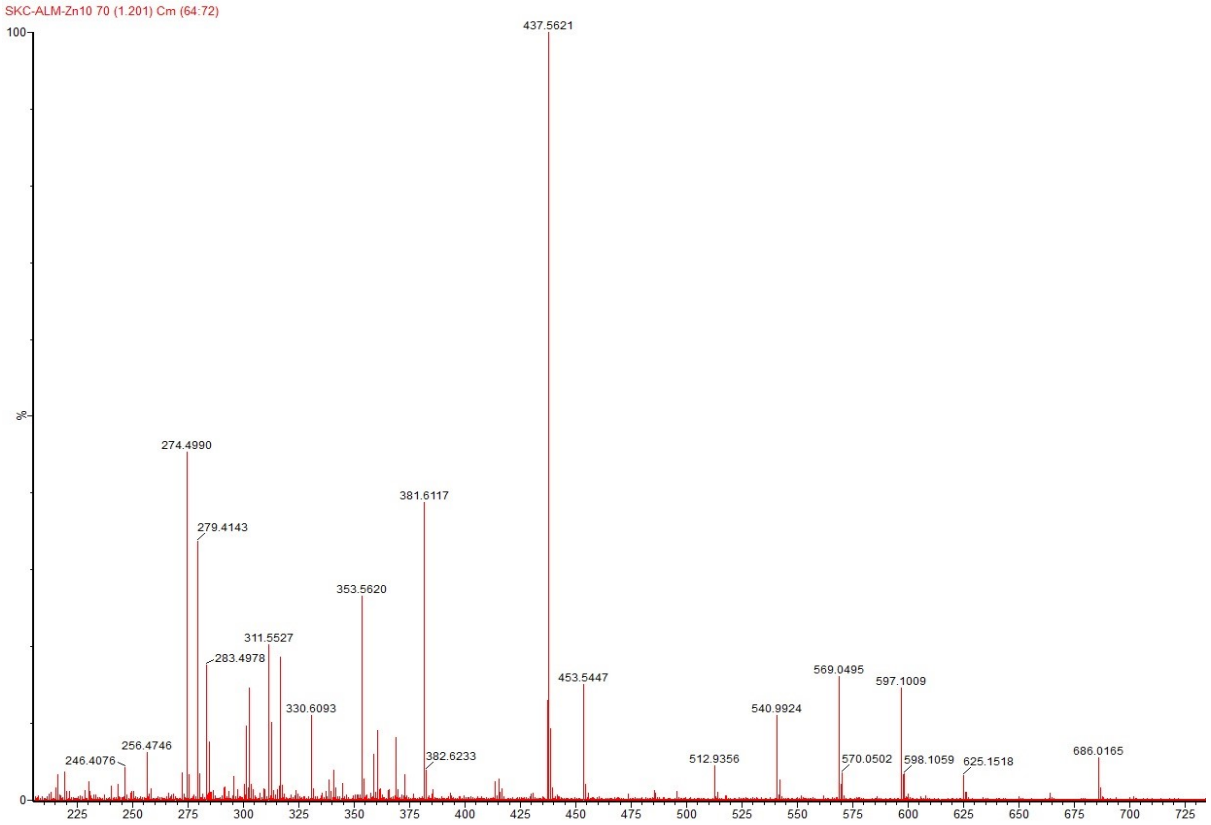

Figure S4. ESI-MS spectrum of complex.

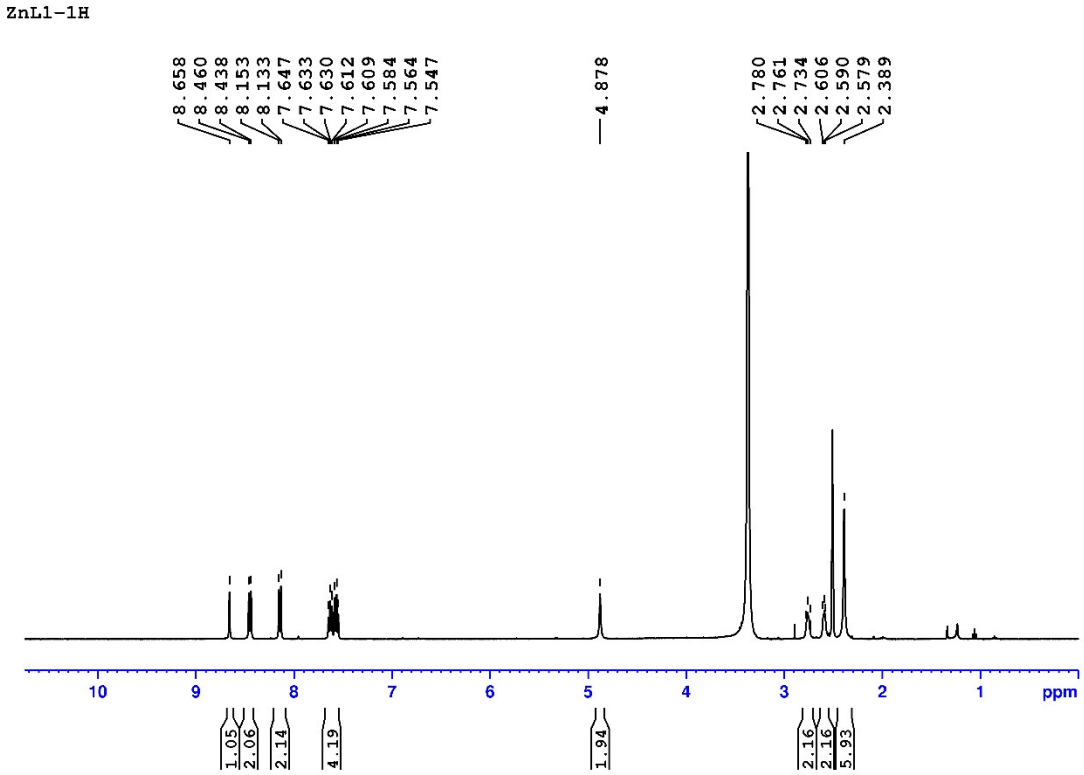

Figure S5. NMR spectrum of complex.

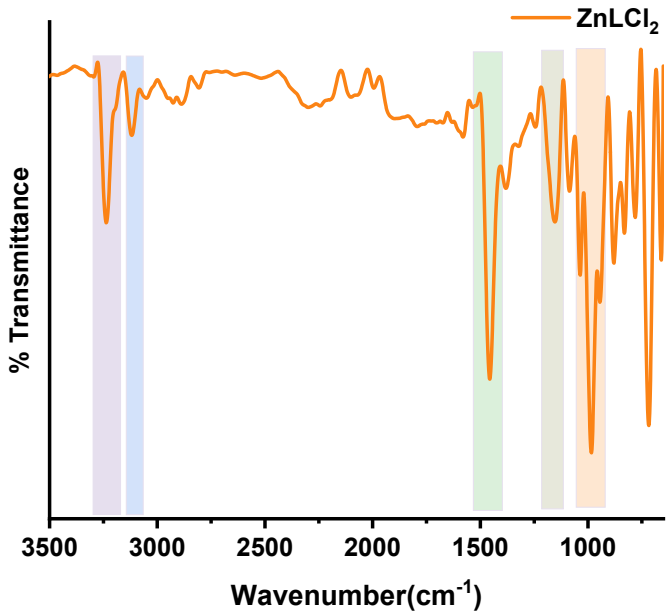

Figure S6. FTIR spectrum of complex.

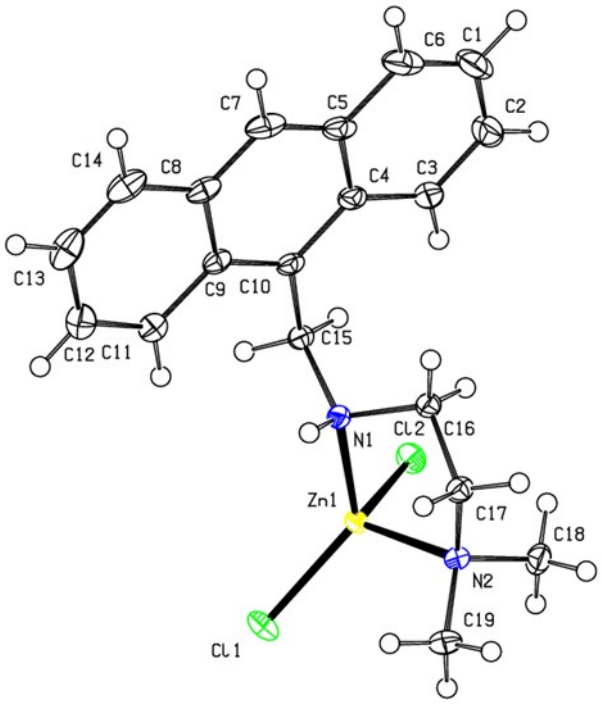

Figure S7. ORTEP diagram of complex at 50 % probability level.

Table S1. X-ray crystallography data of complex

Complex	$ZnLCl_2$
Formula	$C_{19}\ H_{22}\ Cl_2\ N_2\ Zn$
Formula weight	414.65
Crystal size(mm^3)	0.342× 0.226 × 0.147
Temperature	150 K
Crystal system	monoclinic
Space group	P 1 21/c 1
a (Å)	15.3505(10)
b (Å)	11.9330(7)
c(Å)	10.5063(7)
α(°)	90
β(°)	107.988(7)
γ(°)	90
d_{cal}	1.505
Z	4

μ(mm^{-1})	4.554
F*(000)*	856
Total Reflections	13117
Unique Reflections	3693
Observed data [I>2σ(I)]	3504
R(int)	0.029
R1, wR2 [I>2σ(I)]	0.0255, 0.0674
R1, wR2 (all data)	0.0272, 0.0685

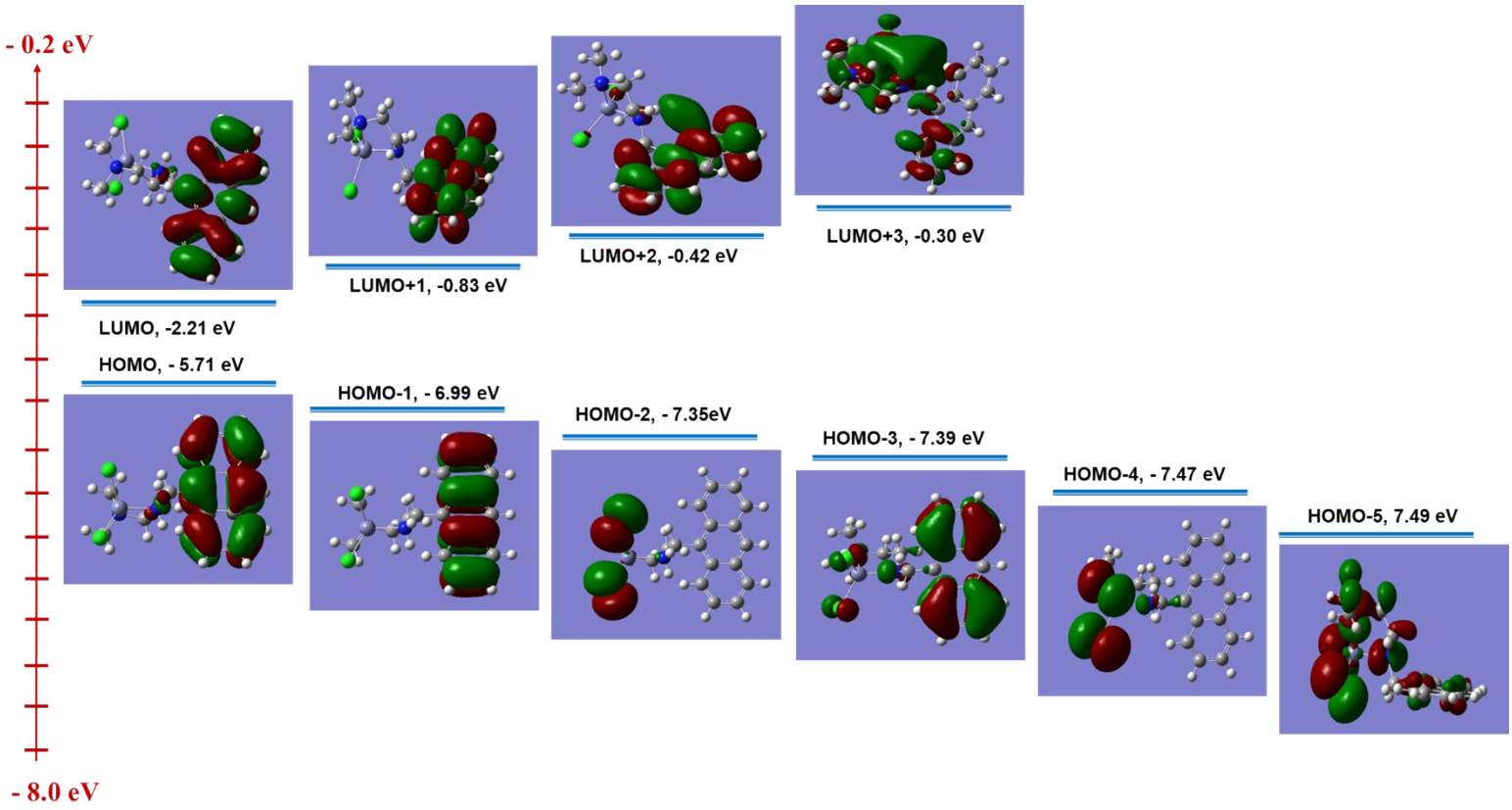

Figure S8. HOMO-LUMO energy diagram of complex.

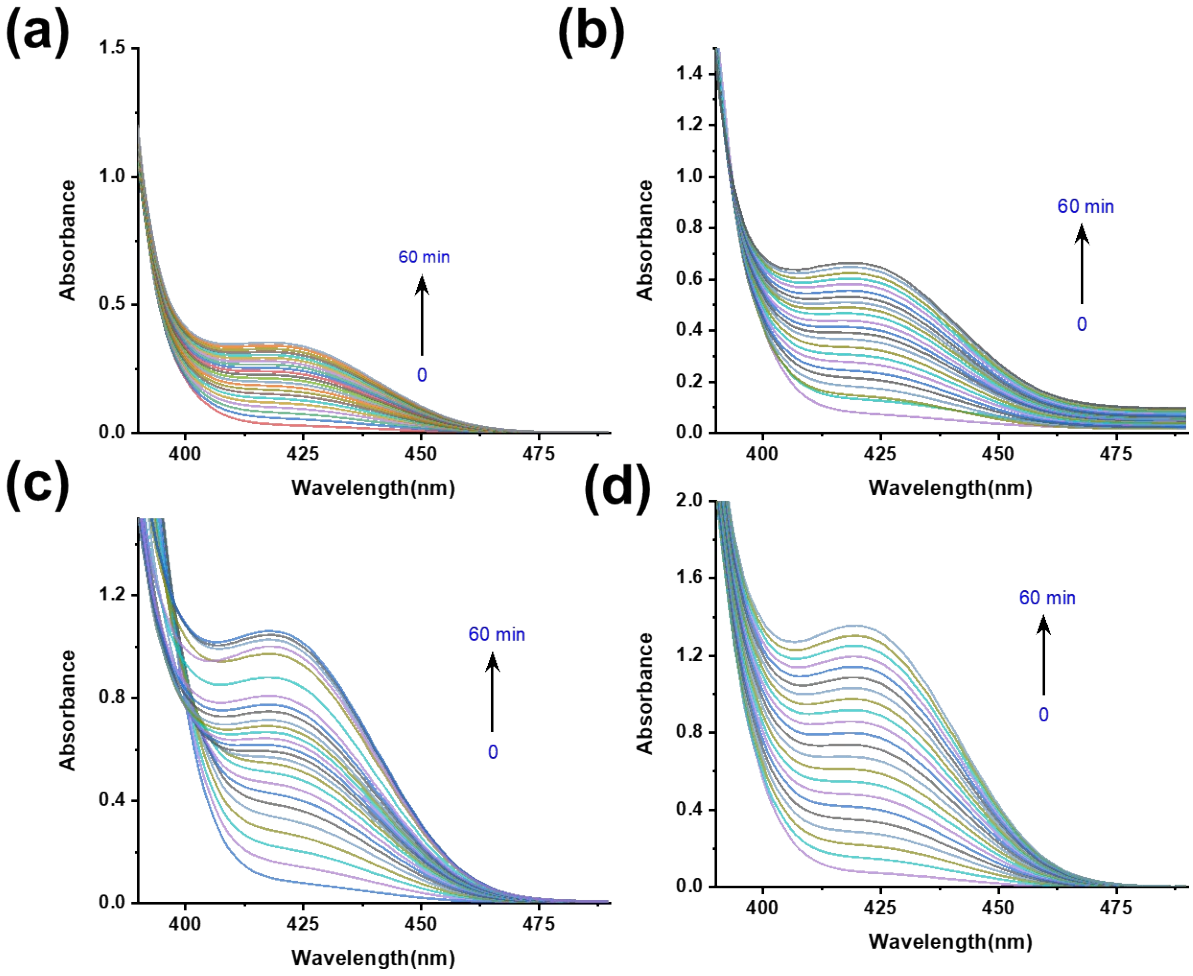

Figure S9. Increase of 4-nitrophenolate band at 421 nm after addition of (a) 20 equiv. (b) 40 equiv. (c) 60 equiv. and (d) 80 equiv. of PNPP to complex solution in DMF/Water medium.

Table S2. Comparison table of phosphatase activity

Complex	**Ligand (L)**	**Substrate for hydrolysis**	**k_{cat} (h^{-1})**	***Ref***
$[ZnLCl_2]$	(N^1-(anthracen-9-ylmethyl)-N^2,N^2-dimethylethane-1,2-diamine)	PNPP	4.78×10^2	*This work*
$[Zn_4(L^1)_4].2H_2O$ $[Zn_2(L^2)_2].2H_2O$	4-(aryl)thiosemicarbazides	PNPP	212(±5) 38(±2)	(Adak et al., 2020)
$[CoL_2Cl_2]$	1,10-phenanthroline	PNPP	3.78×10^2	(Garai et al.,

				2017)
$[Zn_2(L^1)_2X_2]$ $[Zn(HL^2)X_2]$	Mannich-base compartmental ligands	PNPP	4.70×10^4 1.56×10^4	(Sanyal et al., 2015)
$[Zn_2(L^1)_2X_2]$ $[Zn(HL^2)X_2]$	Mannich-base ligands	PNPP	3.36×10^4 7.2×10^3	(Sanyal et al., 2014)
$[Ni_2L^{1-5}(\mu\text{-}NO_3)(NO_3)_2]$	Phenol-based compartmental Mannich-base ligands,	PNPP	$2.16 – 29.2 \times 10^4$	(Sanyal et al., 2016)
$\{[Cu_3(L^1)(NO_3)_2(DMF)(H_2O)]\cdot 3(DMF)\}_n$ $[Cu_3(L^1)(Cl)_2(DMF)_2]_n$ $[Cu_3(L^2)(NO_3)_4(H_2O)_4]_n$	one-dimensional coordination polymer	HNPP	34.56	(Hussain et al., 2016)
$[Cu_2(ccdp)(\mu\text{-}OAc)]^{2-}$ $[Zn_2(ccdp)(\mu\text{-}OAc)]^{2-}$	Carboxylate-rich ligand H_5ccdp (N,N′-Bis[2-carboxybenzomethyl]-N,N′-Bis[carboxymethyl]-1,3-diaminopropan-2-ol)	PNPP; (pH 8, 37 °C) BNPP ; (pH 9, 37 °C)	8.42×10^{-3} 1.67×10^{-4}	(Foley et al., 2021)
$[Zn_2(L^1)(\mu\text{-}OAc)_2]^{2+}$	2,6-bis{[bis(2-pyridylmethyl)amino]methyl}-4-t-butylphenoxide	BDNPP	1.152	(Pathak et al., 2018)

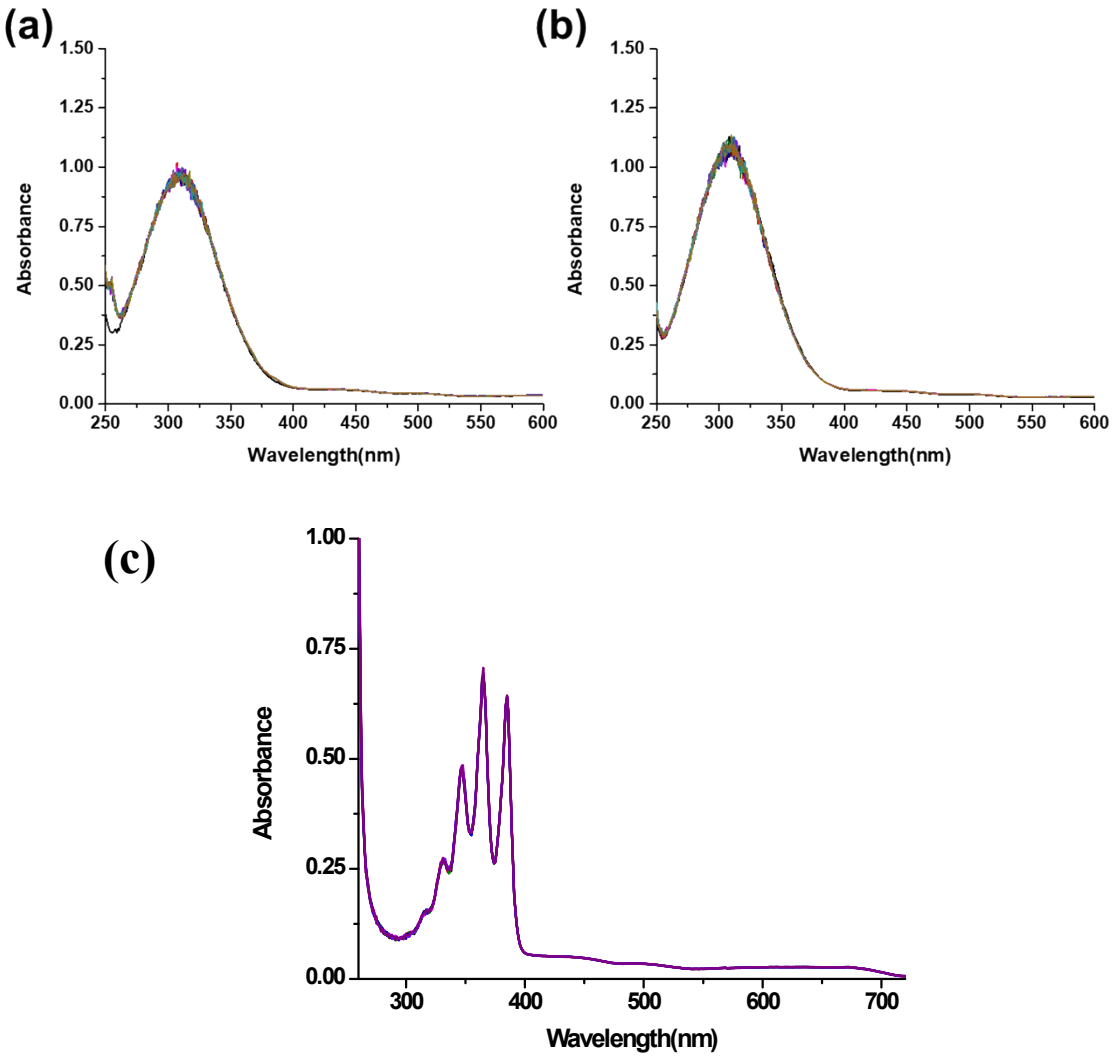

Figure S10. Time-dependent spectra of PNPP (a) in presence of ligand and (b) in presence of $ZnCl_2$; (c) time dependent spectra of the complex over a period of 5 h at 30 min intervals.

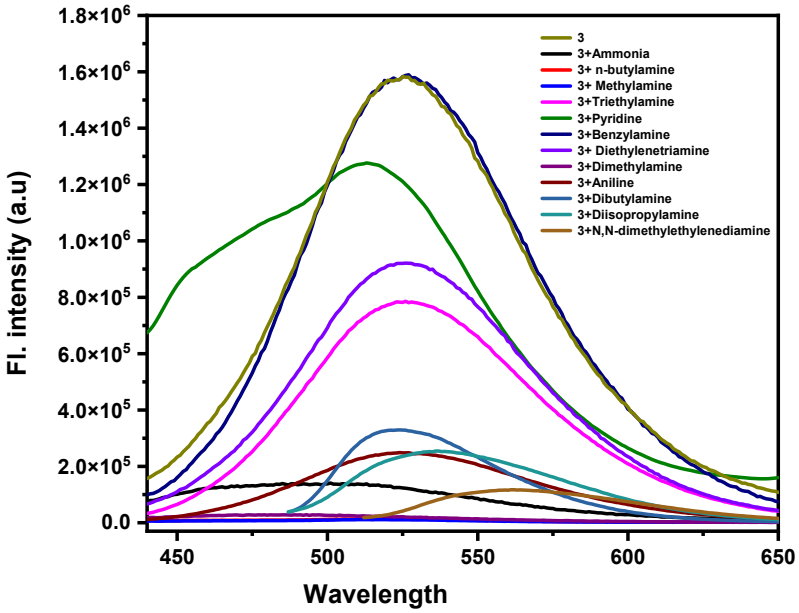

Figure S11. Solid state emission spectra of complex in presence of different amine vapors at 35 °C.

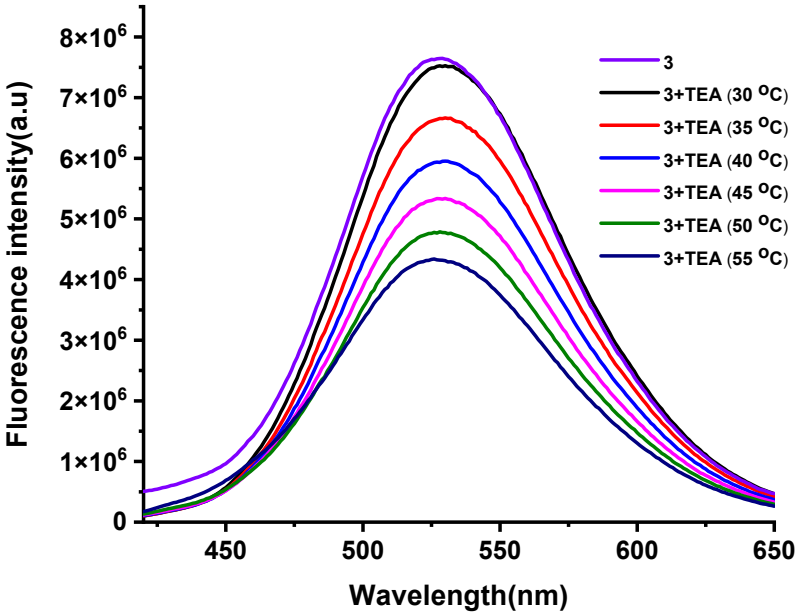

Figure S12. Solid state emission spectra of the complex in presence of triethylamine vapour at different temperature.

Reference:

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