

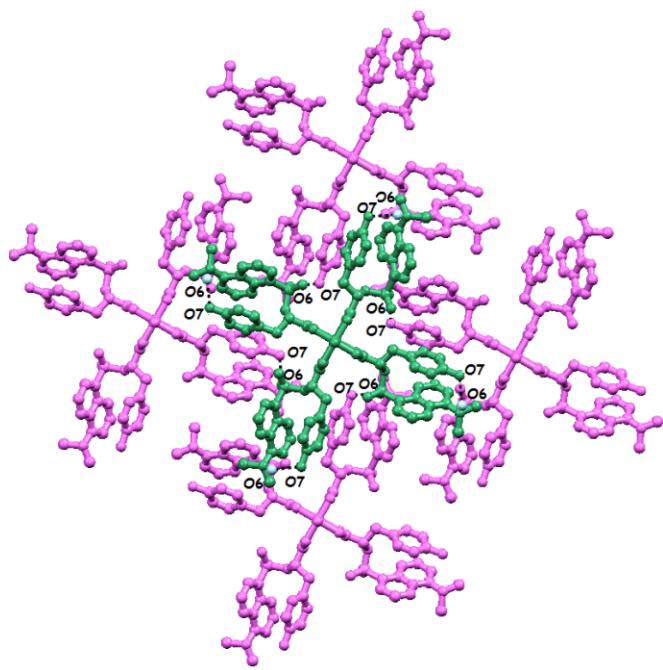
## A homochiral luminescent compound with four-fold symmetry as a potential chemosensor for nitroanilines

Navnita Kumar<sup>a</sup>, Sadhika Khullar<sup>ab</sup> and Sanjay K. Mandal<sup>\*a</sup>

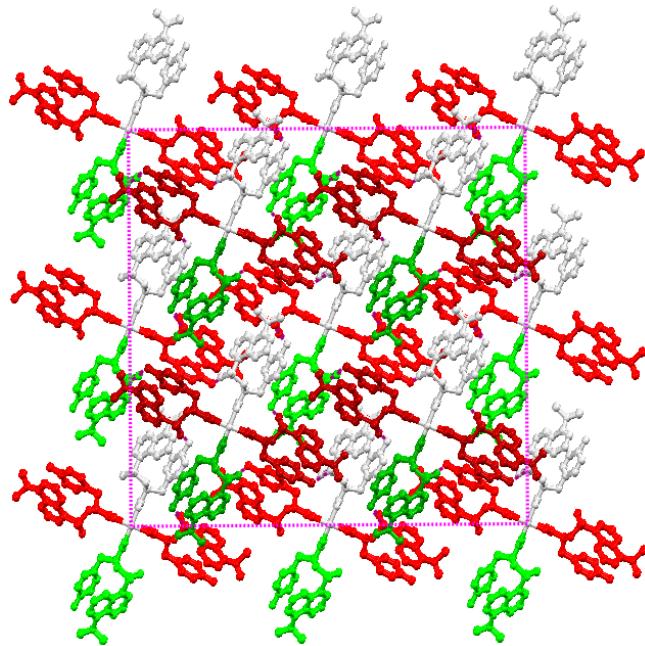
<sup>a</sup>Department of Chemical Sciences, Indian Institute of Science Education and Research, Mohali, Sector 81, Manauli PO, S.A.S. Nagar, Mohali (Punjab) 140306, INDIA

<sup>b</sup>Department of Chemistry, DAV University, Jalandhar, Punjab 144001, INDIA  
\*e-mail: sanjaymandal@iisermohali.ac.in

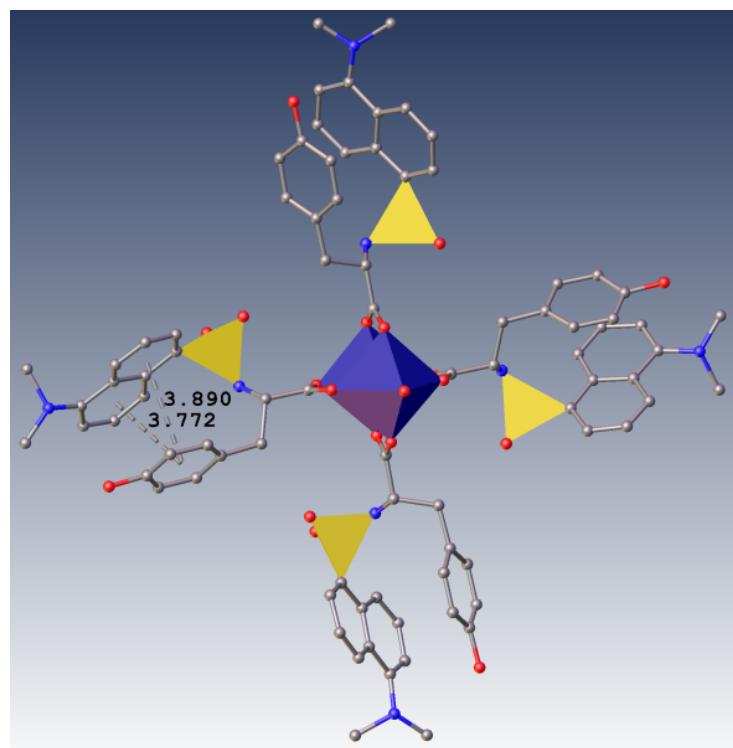
## Supplementary Information



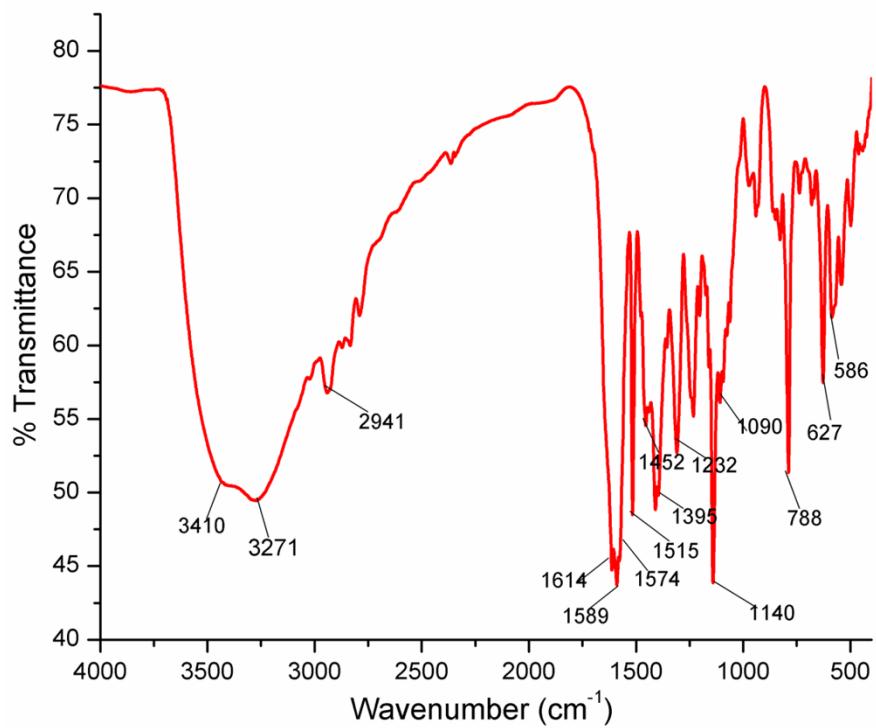
**Fig. S1** Dinuclear subunit surrounded by four other dinuclear subunits.



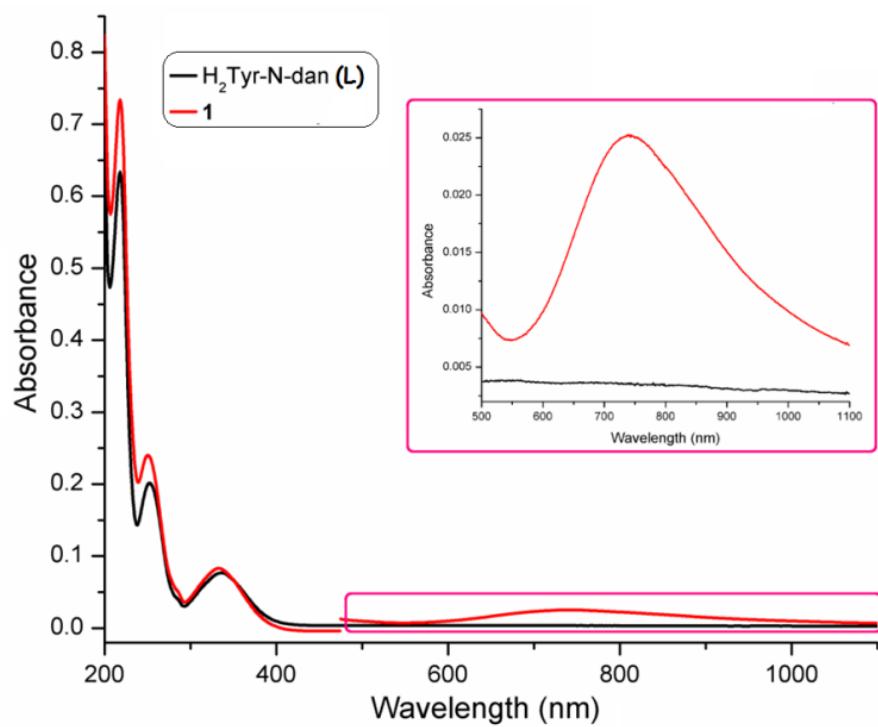
**Fig. S2** Growth of the square synthon (different colors represent the symmetry operations).



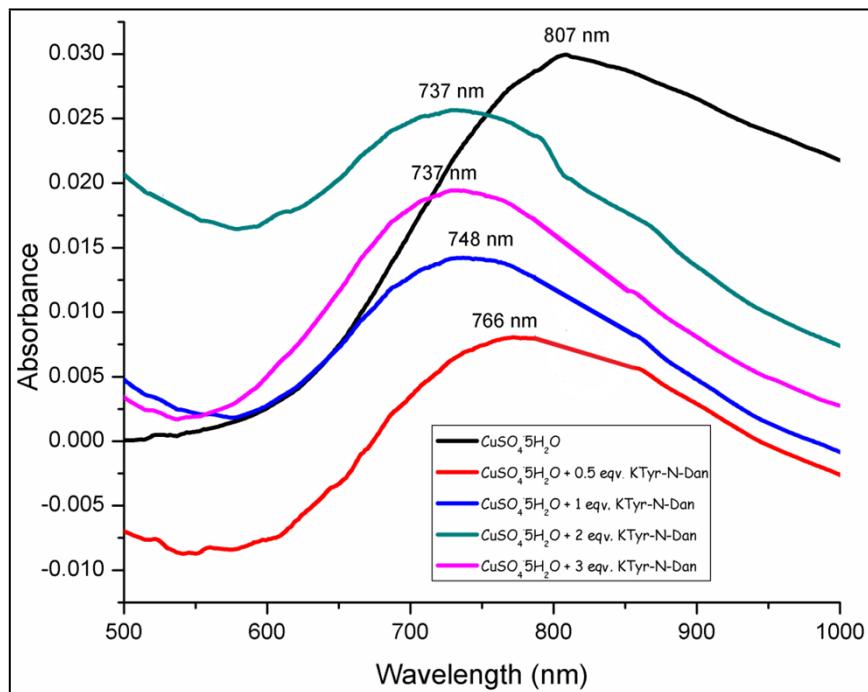
**Fig. S3** Schematic view showing  $\pi-\pi$  interactions in **1**.



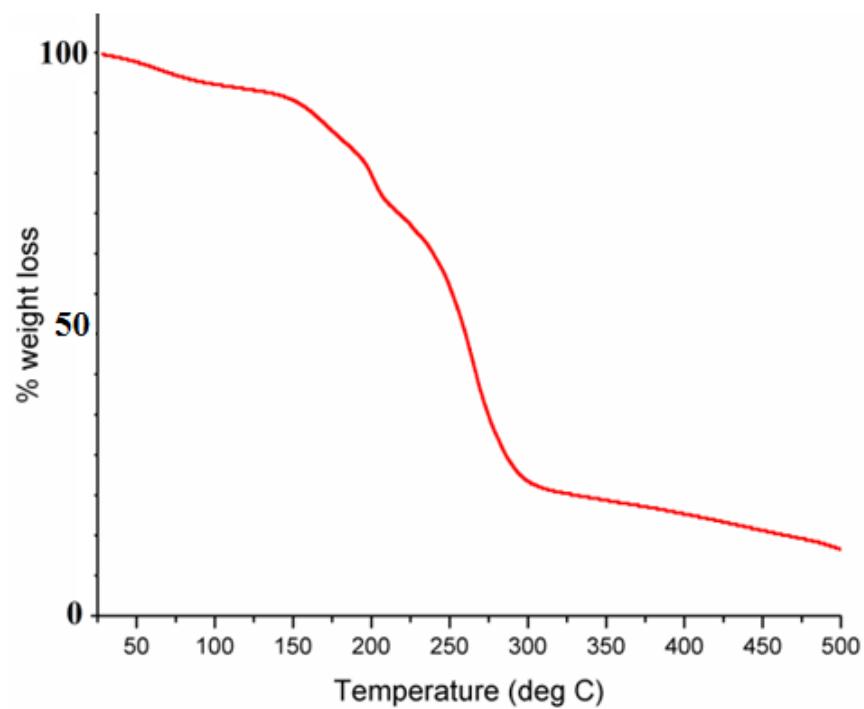
**Fig. S4** IR spectrum of **1**.



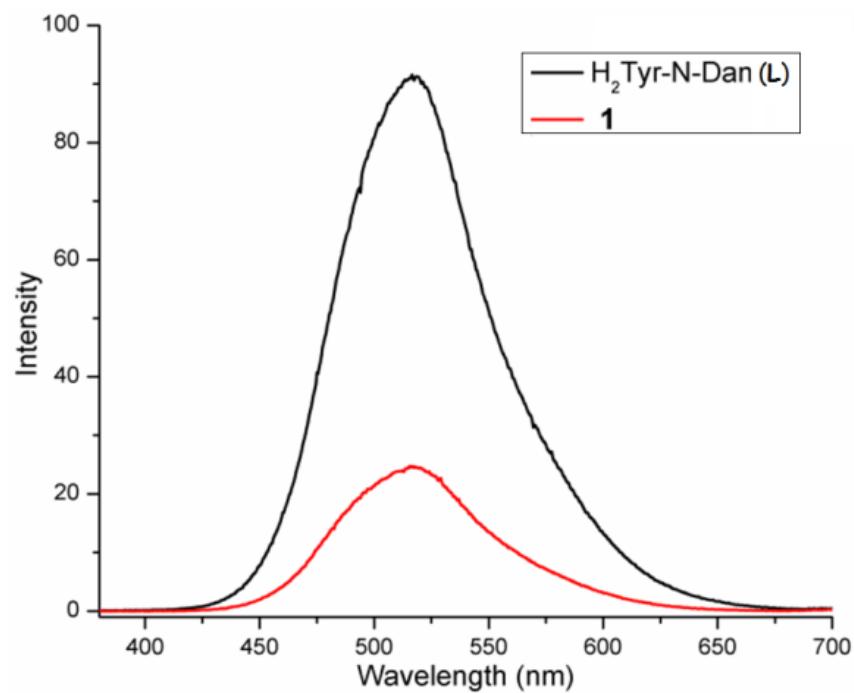
**Fig. S5** UV-Visible absorbance spectra of ligand and **1**. Inset: Absorbance in the visible region.



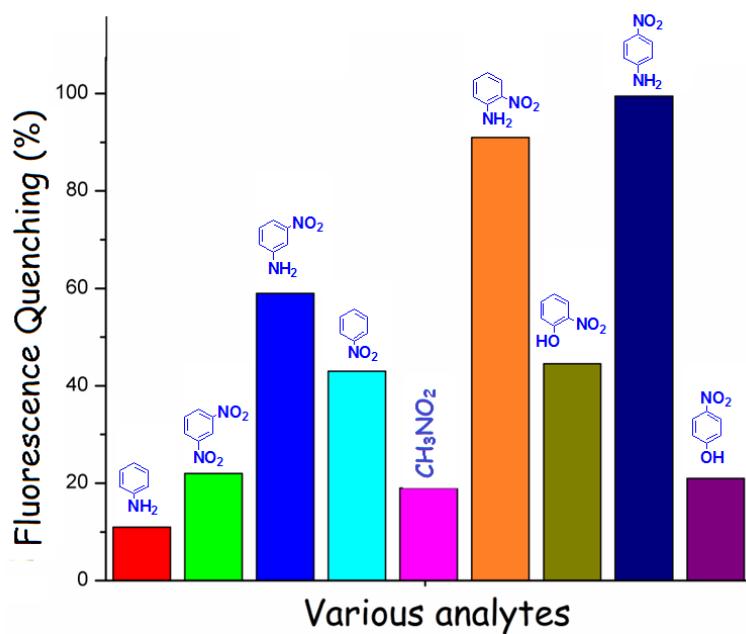
**Fig. S6** Monitoring the formation of **1** from  $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$  and Ktir-N-Dan in methanol by UV-Visible spectroscopy.



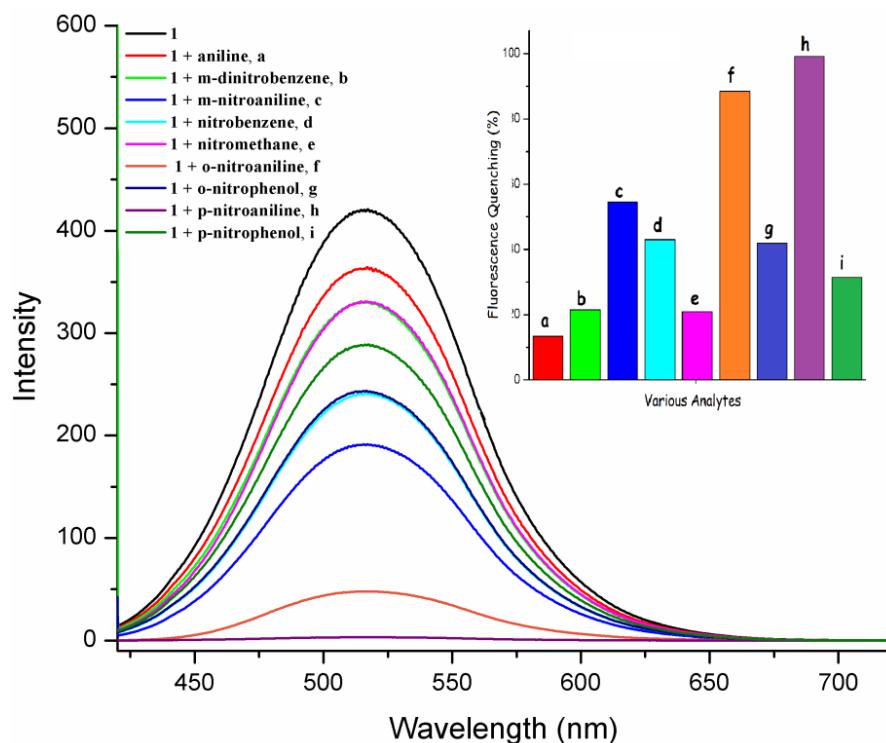
**Fig. S7** TGA scan for **1**.



**Fig. S8** Photoluminescence spectra for  $\text{H}_2\text{Tyr-N-Dan}$  and **1**.



**Fig. S9** Comparative study of the role various analytes on quenching the fluorescence intensity of ligand in methanol .



**Fig. S10** Change in Fluorescence intensity for complex **1** in methanol upon addition of various analytes.

**Table S1.** Selected bond lengths ( $\text{\AA}$ ) and bond angles (degrees) in **1**.

Cu1-O4 <sup>#1</sup>	1.949(4)	Cu1-O4 <sup>#3</sup>	1.949(4)
Cu1-O4 <sup>#2</sup>	1.949(4)	Cu1-O4	1.949(4)
Cu1-O1	2.130(10)	Cu1-Cu2	2.6384(14)
Cu2-O3 <sup>#1</sup>	1.968(4)	Cu2-O3 <sup>#2</sup>	1.968(4)
Cu2-O3 <sup>#3</sup>	1.968(4)	Cu2-O3	1.968(4)
Cu2-O2	2.161(11)		

O4 <sup>#1</sup> -Cu1-O4 <sup>#3</sup>	89.47(3)	O4#1-Cu1-O4#2	89.47(3)
O4 <sup>#3</sup> -Cu1-O4 <sup>#2</sup>	168.9(3)	O4 <sup>#1</sup> -Cu1-O4	168.9(3)
O4 <sup>#3</sup> -Cu1-O4	89.47(3)	O4 <sup>#2</sup> -Cu1-O4	89.47(3)
O4 <sup>#1</sup> -Cu1-O1	95.53(15)	O4 <sup>#3</sup> -Cu1-O1	95.53(15)
O4 <sup>#2</sup> -Cu1-O1	95.53(15)	O4-Cu1-O1	95.53(15)
O4 <sup>#1</sup> -Cu1-Cu2	84.47(15)	O4 <sup>#3</sup> -Cu1-Cu2	84.47(15)
O4 <sup>#2</sup> -Cu1-Cu2	84.47(15)	O4-Cu1-Cu2	84.47(15)
O1-Cu1-Cu2	180.000(2)	O3 <sup>#1</sup> -Cu2-O3 <sup>#2</sup>	89.33(3)
O3 <sup>#1</sup> -Cu2-O3 <sup>#3</sup>	89.33(3)	O3 <sup>#2</sup> -Cu2-O3 <sup>#3</sup>	167.6(3)
O3 <sup>#1</sup> -Cu2-O3	167.6(3)	O3 <sup>#2</sup> -Cu2-O3	89.33(3)
O3 <sup>#3</sup> -Cu2-O3	89.33(3)	O3 <sup>#1</sup> -Cu2-O2	96.21(13)
O3 <sup>#2</sup> -Cu2-O2	96.21(13)	O3 <sup>#3</sup> -Cu2-O2	96.21(13)
O3-Cu2-O2	96.21(13)	O3 <sup>#1</sup> -Cu2-Cu1	83.79(13)
O3 <sup>#2</sup> -Cu2-Cu1	83.79(13)	O3 <sup>#3</sup> -Cu2-Cu1	83.79(13)
O3-Cu2-Cu1	83.79(13)	O2-Cu2-Cu1	180.000(2)
C1-O3-Cu2	122.3(3)	C1-O4-Cu1	122.6(4)

Symmetry transformations used to generate equivalent atoms:

#1	-x+2, -y+2, z
#2	x+2, -y, z
#3	-x, y+2, z