Supporting information.

Imine linked fluorescent covalent organic cage: sensing of chloroform vapour, metal ions and detection of nitroaromatics.

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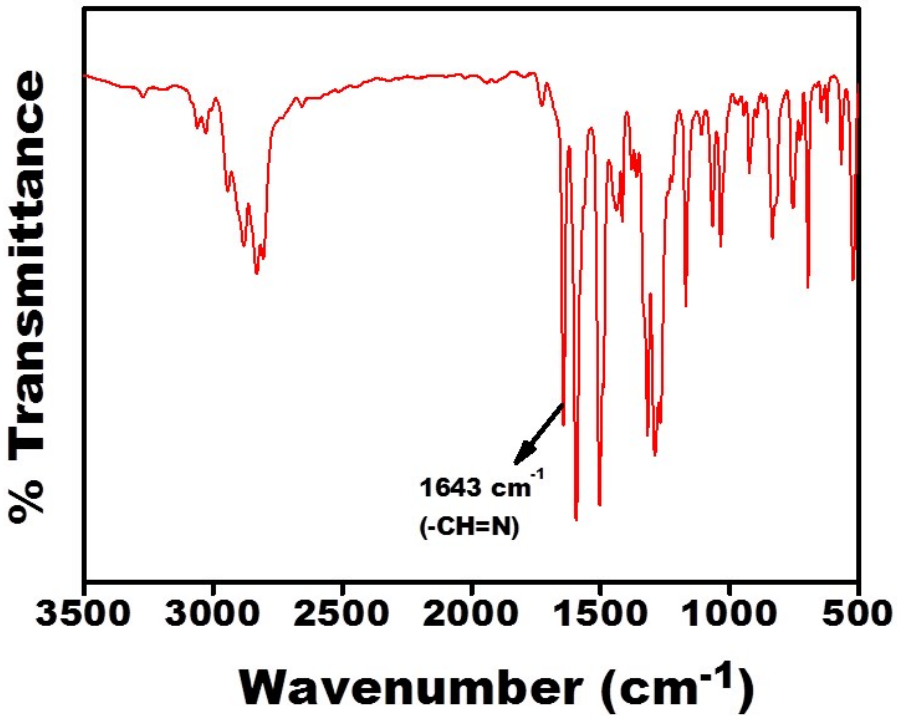

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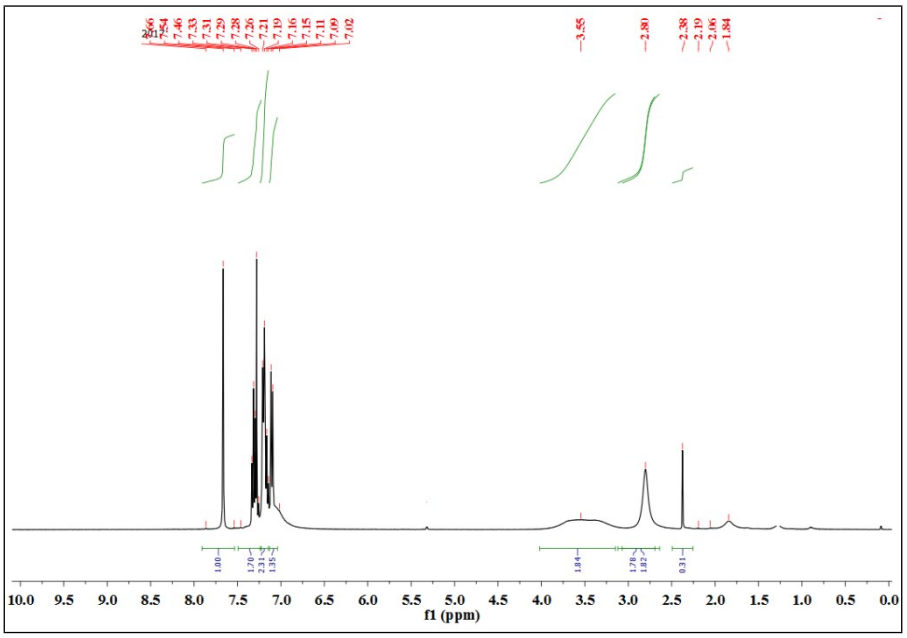

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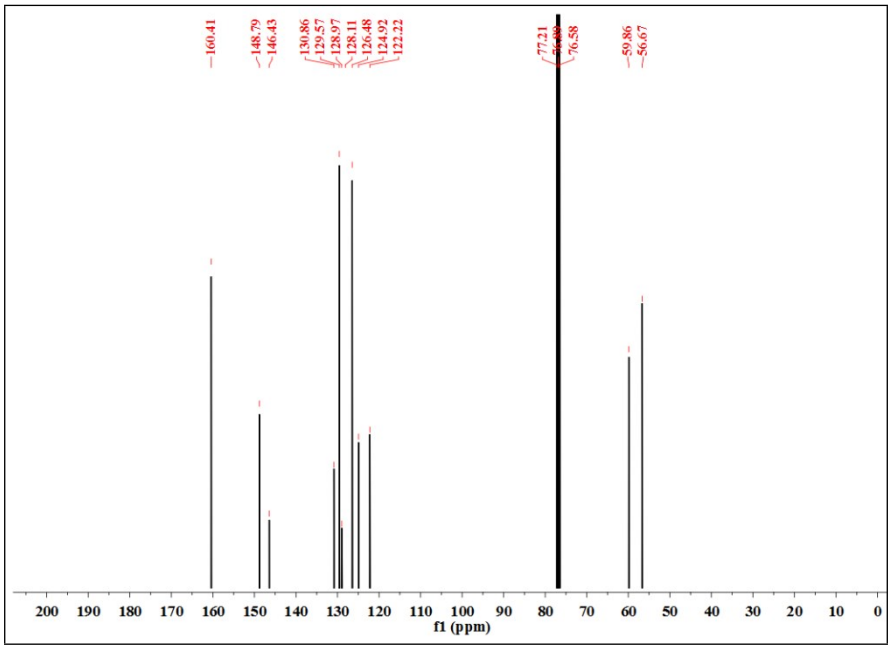

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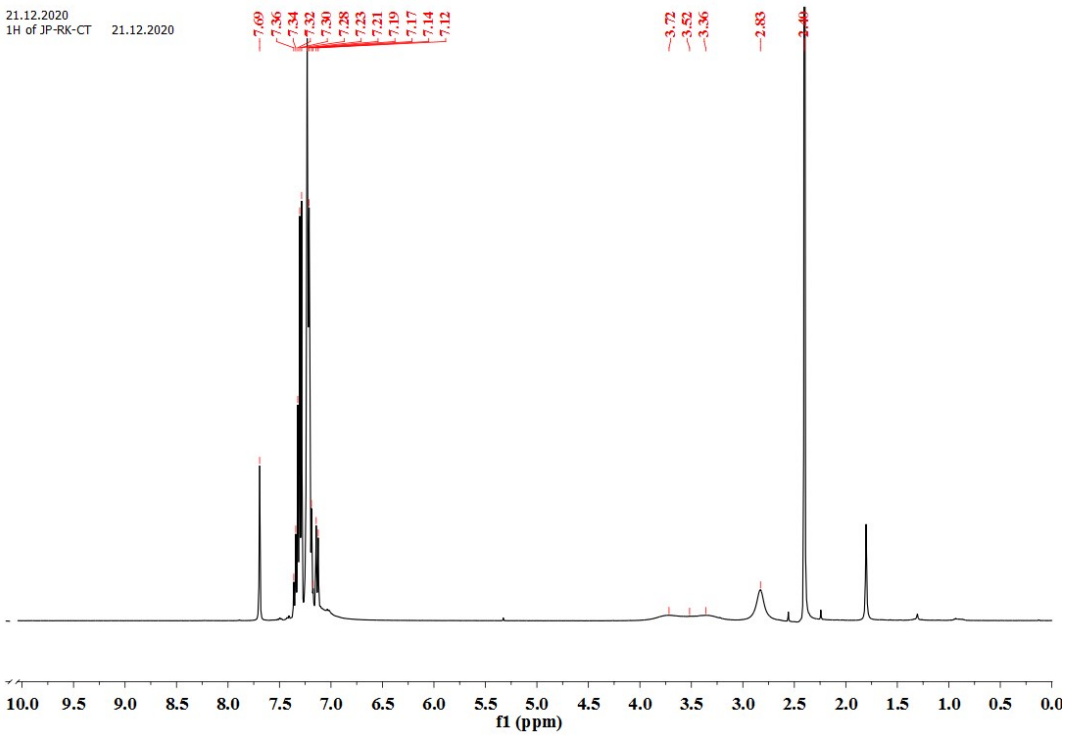

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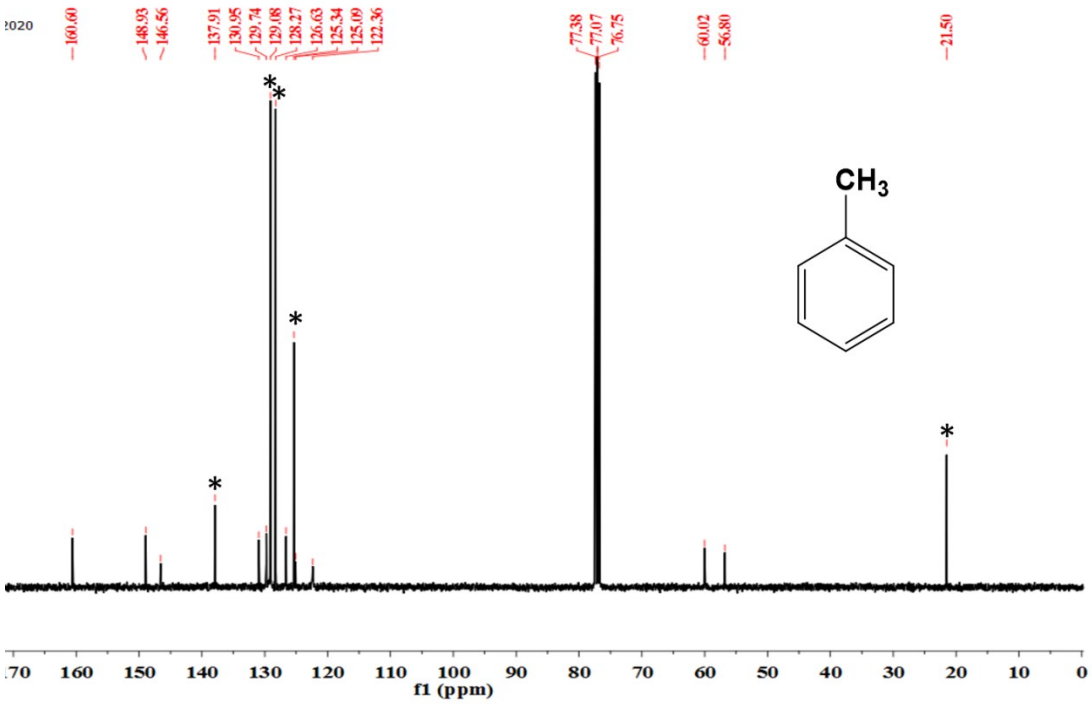

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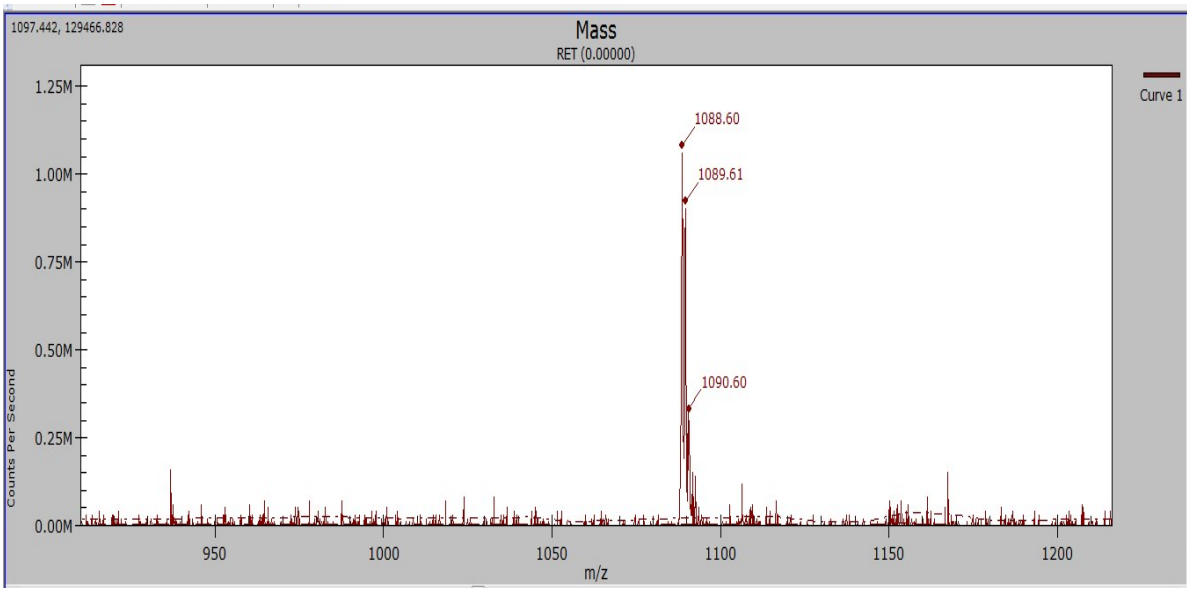

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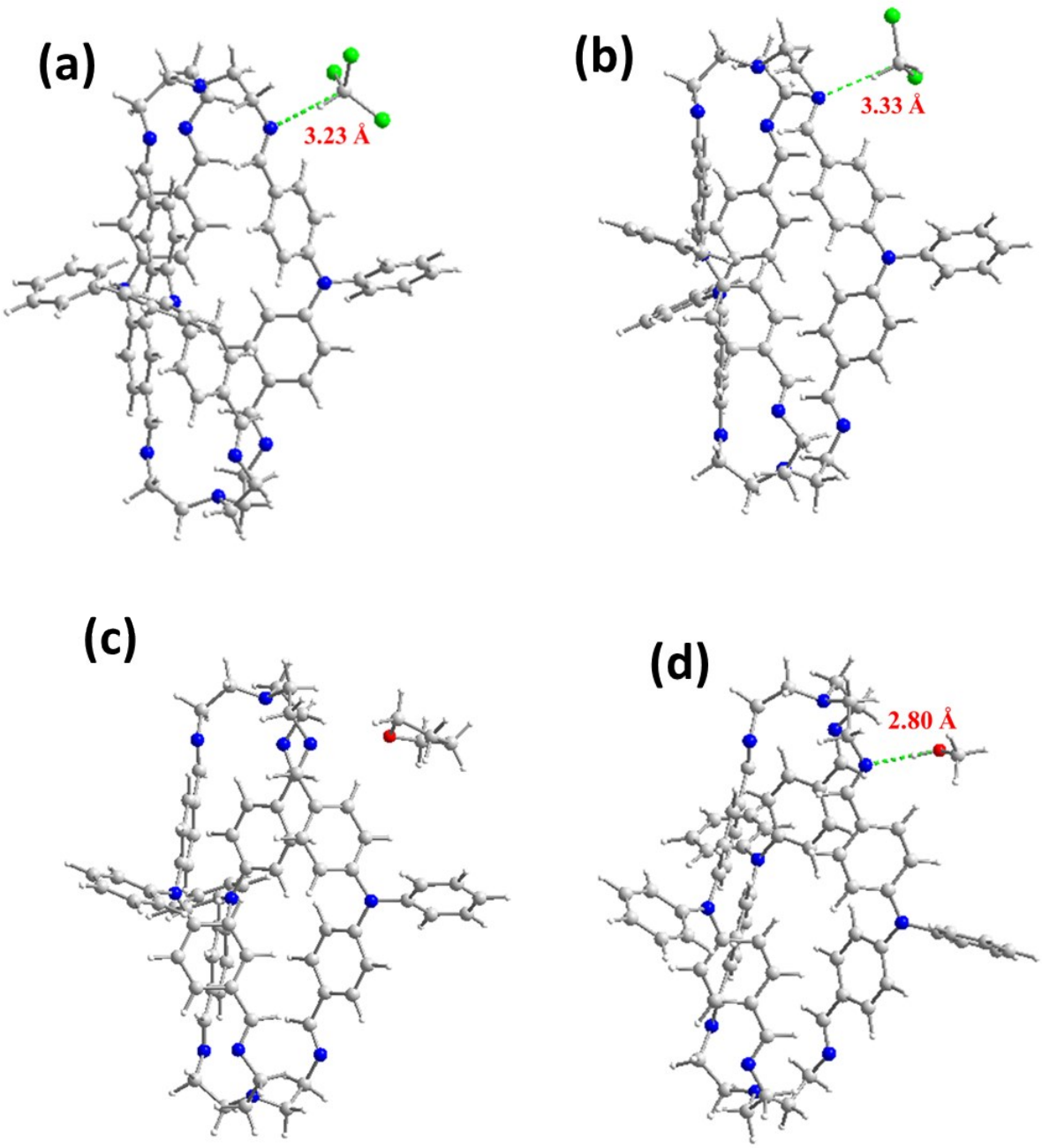

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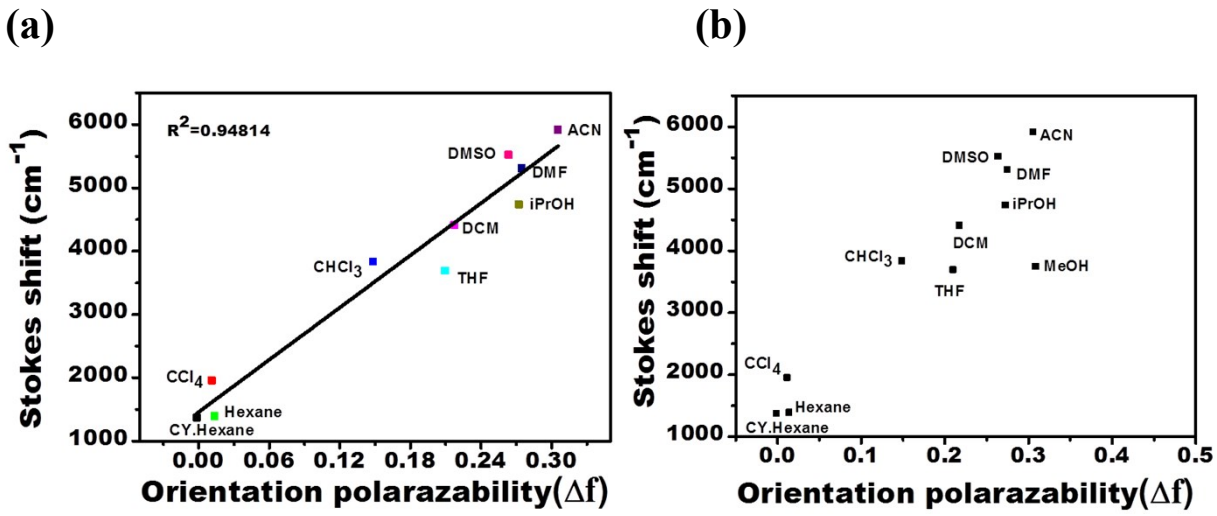

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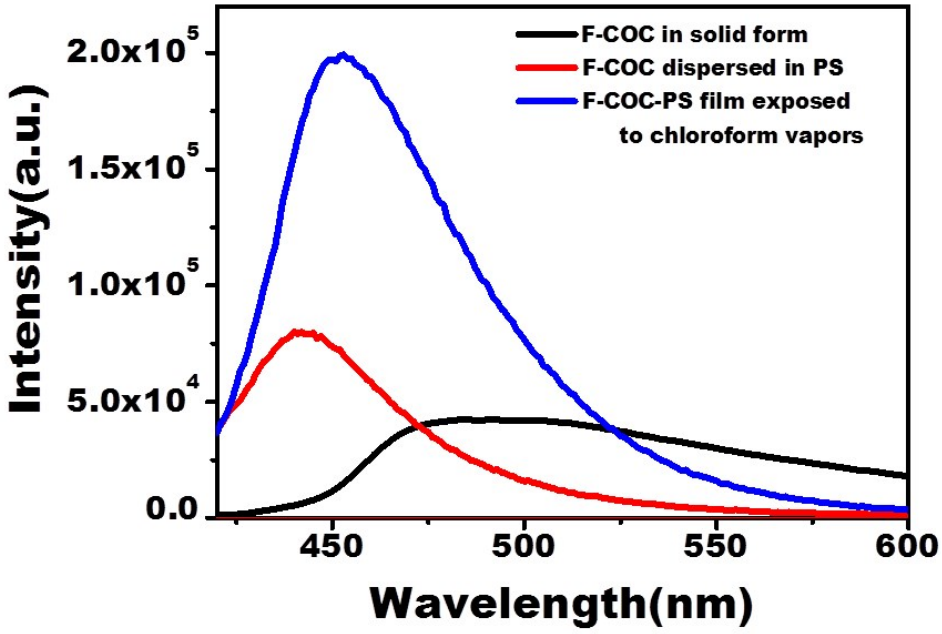

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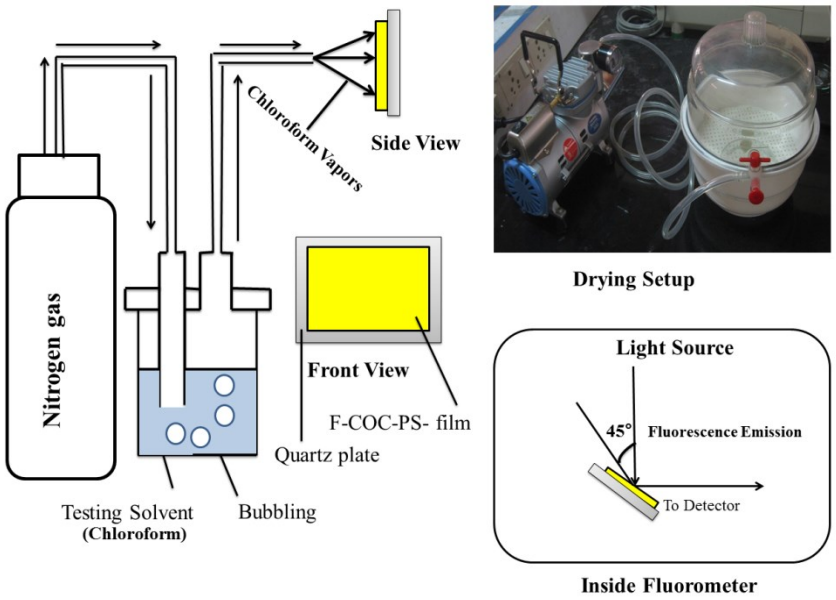

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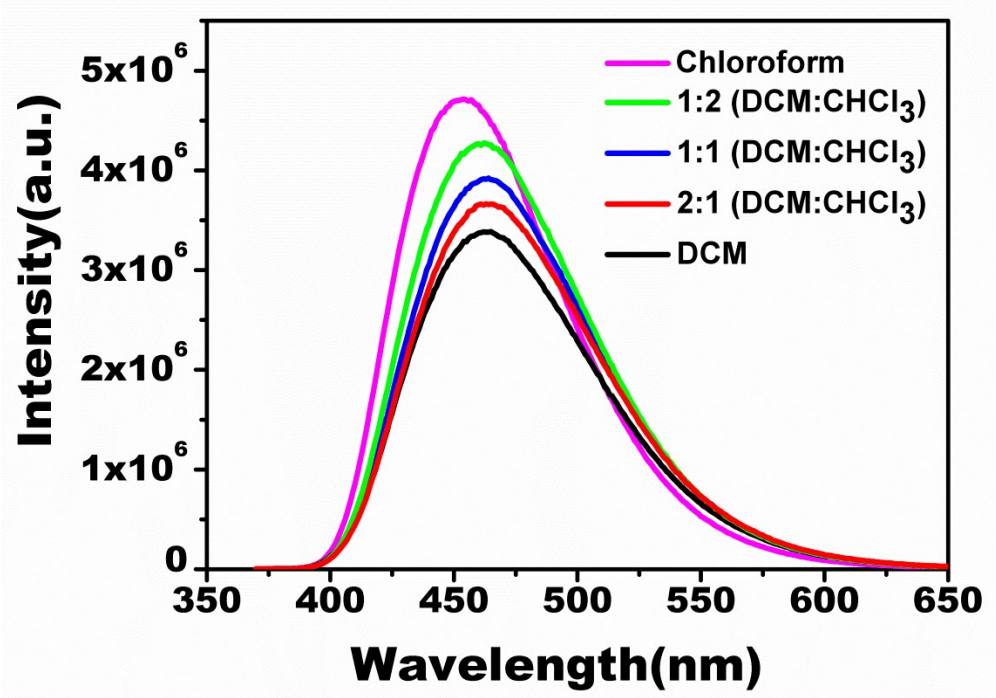
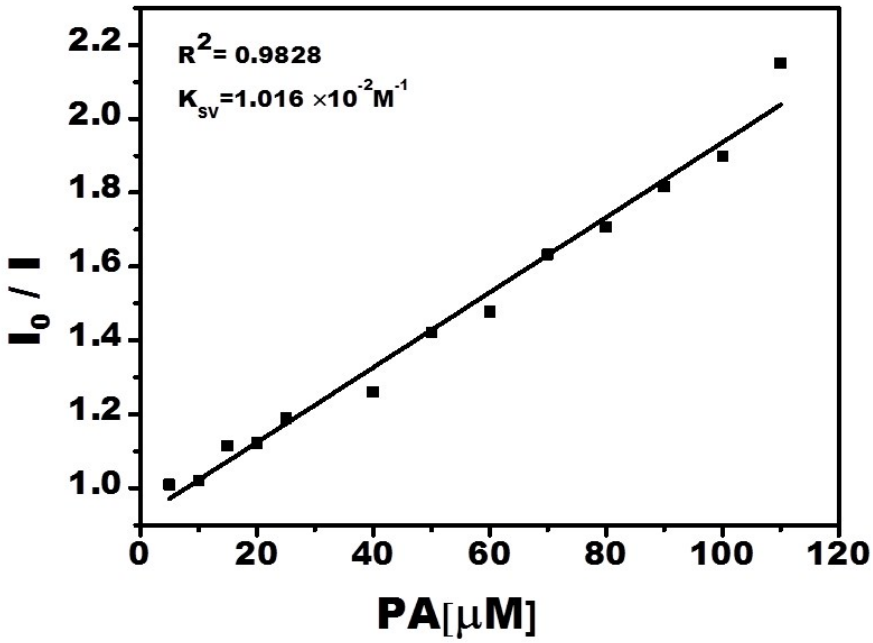


Fig. S11: Fluorescence emission spectra of F-COC cage in $CHCl_3$ and DCM solvent mixture in various rations.



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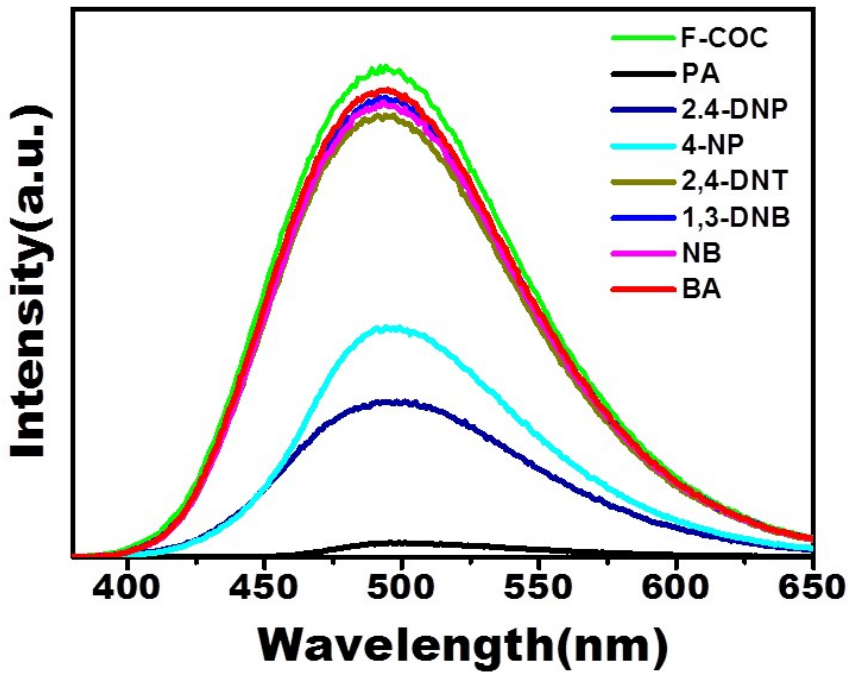


Fig. S13: Fluorescence emission of F-COC with different nitro analytes.

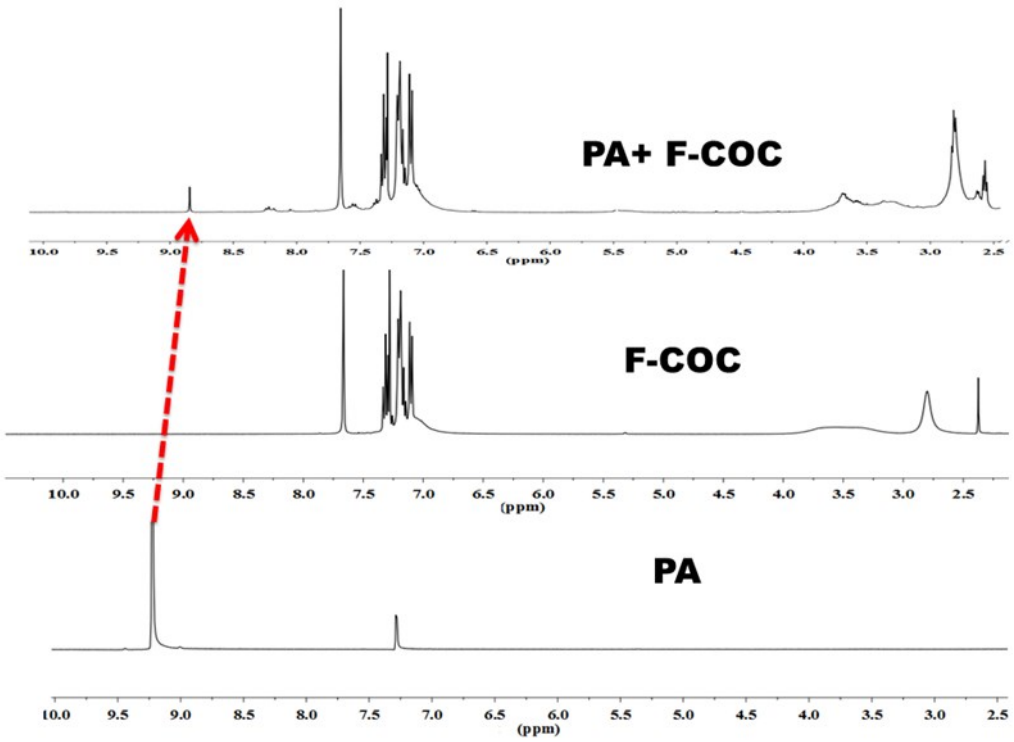


Fig. S14: ^{1}H NMR spectra of F-COC before and after addition of PA recorded in $CDCl_3$ (Red arrow indicating the change in chemical shift of PA acidic proton towards up field).

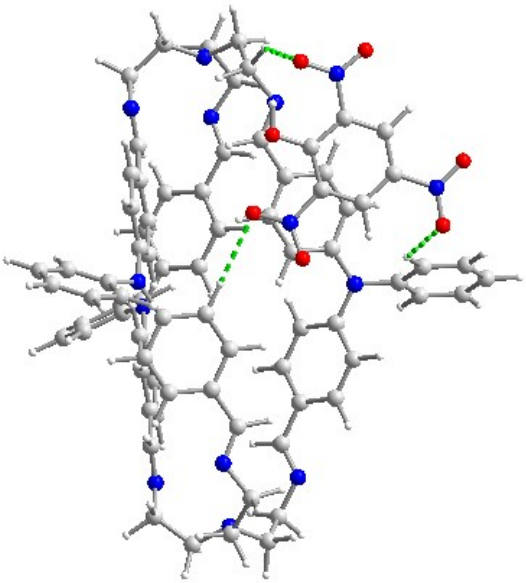


Fig. S15: Hydrogen bonding interactions observed in the optimized geometries of the F-COC with PA.

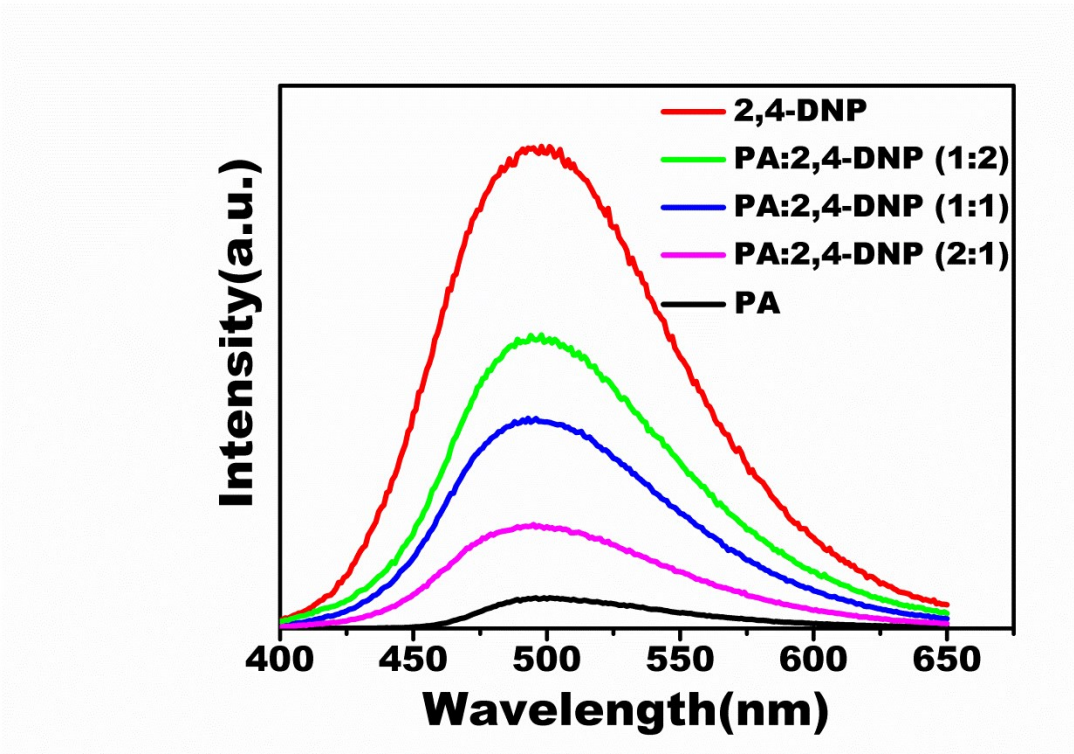


Fig. S16: Fluorescence emission plots of F-COC in DMSO solutions of mixture of picric acid and 2,4-DNP in various rations.

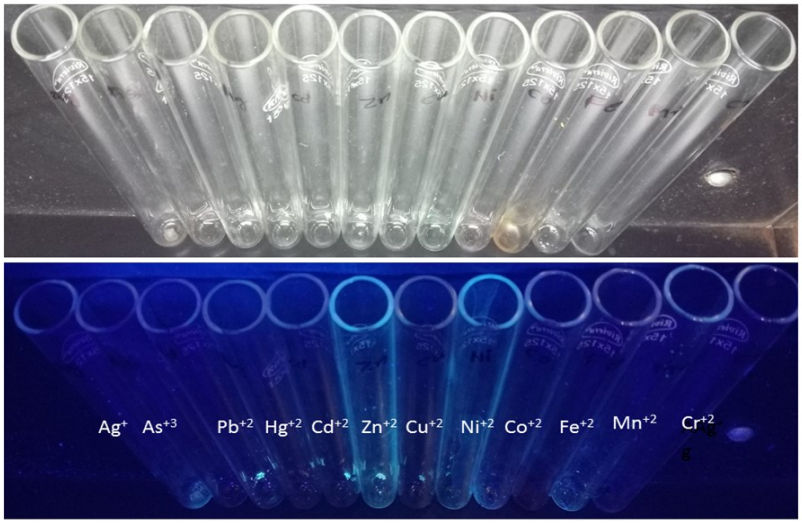


Fig. S17: Solid samples of F-COC cage coordination complexes with different metal ions viewing in normal visible light (Top). (b) Under UV light at 365 nm (down).

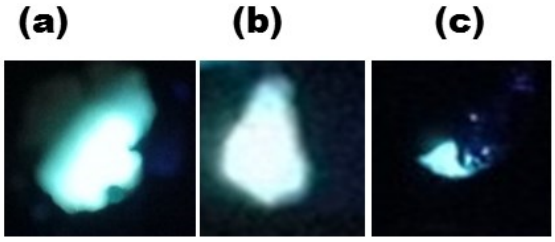
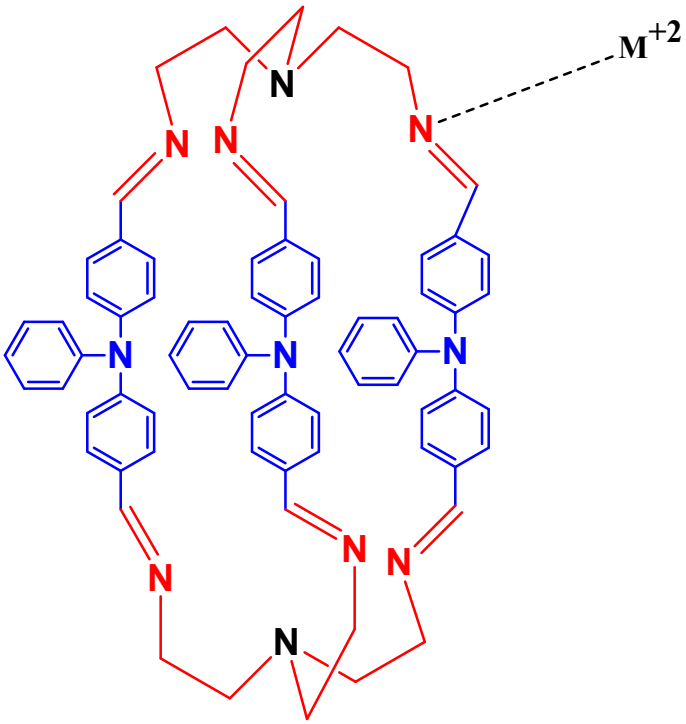


Fig. S18: Photographs of (a) Zn^{+2} – F-COC (b) Cd^{+2} - F-COC (c) Pb^{+2} – F-COC coordination complexes in powder form under UV light at 365 nm.



M^{+2} = Zn^{+2}, Cu^{+2}, Pb^{+2}, Cd^{+2}

Fig. 19: Schematic representation of Coordination mode of F-COC with metal ions.

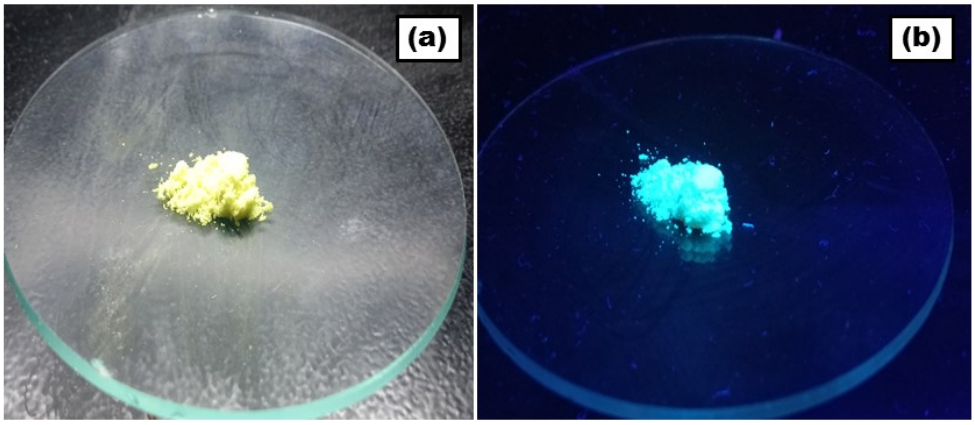


Fig. S20: Digital photograph of the solid F-COC in powder form under (a) normal light (b) UV light at 365 nm.

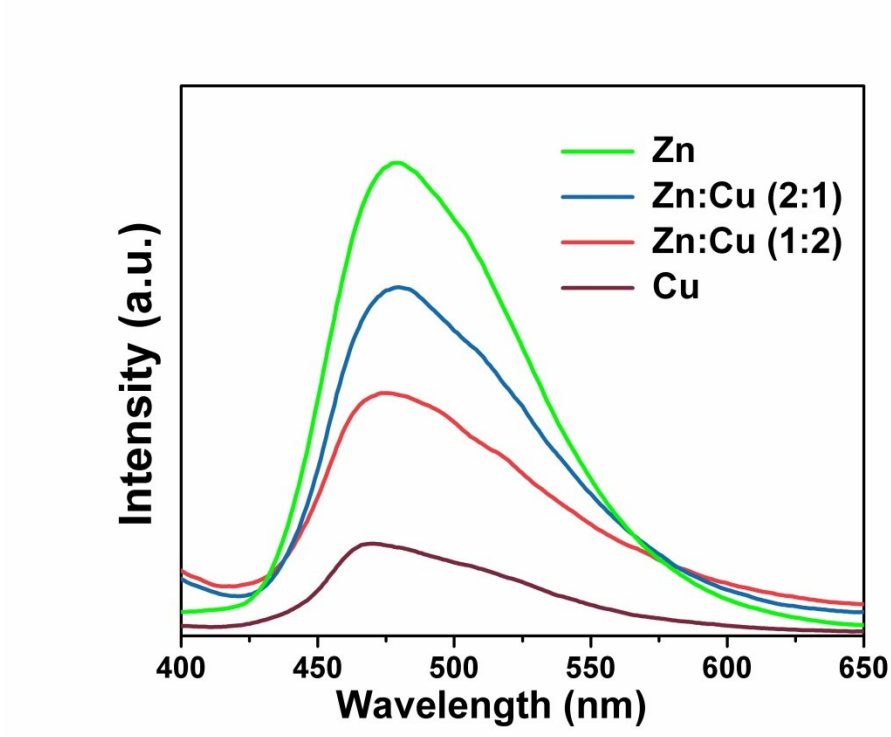


Fig. S21: PL emission spectra of F-COC with Zn^{+2} and Cu^{+2} metal ions in various rations in solid state.

Table. S1: Single crystal data information of F-COC crystal.

Compound	COC-1
Formula	$C_{77}H_{69}N_{11}$
mw [g.mol^{-1}]	1148.43
space group, Z	*P -1*, 2
***a* (Å)**	13.0867(11)
***b* (Å)**	13.5562(13)
***c* (Å)**	20.724(2)
***α* (°)**	87.641(5)
***β* (°)**	83.468(5)
***γ* (°)**	61.366(4)
***V* (Å^3)**	3205.5(5)
radiation, λ (Å)	Mo Kα, 0.71073
ρ_{calcd} (g·cm^{-3})	1.190
μ (mm^{-1})	0.071
R1/wR2,[a] $I \geq 2\sigma_I$	0.0845, 0.2002
R1/wR2,[a] all data	0.1745, 0.2454

Table. S2: Observed and calculated absorption maxima of high energy absorption band of F-COC observed at around 360 nm.

S. No.	**Solvent Name**	**Absorption max. Wavelength (λ_{max}) (nm)**	
		Observed	**Calculated**
1	hexane	**326**	**322.3**
2	cy-hexane	**326**	**322.6**
3	CCl4	**331**	**322.4**
4	chloroform	**332**	**327**
5	THF	**328**	**325.8**
6	DCM	**332**	**326.1**
7	iso-proponol	**328**	**326.8**
8	methanol	**328**	**327.1**
9	DMF	**328**	**327.3**
10	acetonitrile	**325**	**327.4**
11	DMSO	**331**	**327.4**

Table. S3: Spectral data of F-COC in various solvents.

Solvent	**E_T (30) (kcal.mol^{-1})**	**λ_{abs} (nm)**	**λ_{em} (nm)**	**$\Delta\bar{\nu}$ (cm^{-1})**	**Δf (cm^{-1})**
Acetonitrile	45.6	375	482	5919.8	0.3054
Chloroform	39.1	383	449	3837.9	0.1482
CCl_4	32.4	377	407	1955.2	0.0112
Chlorobenzene	37.5	381	436	3310.9	0.142
Cyclohexane	30.9	372	392	1371.5	-0.0016
1,2-DCE	41.9	381	462	4601.6	0.2208
DCM	40.7	381	458	4412.7	0.2171
1,4-Dioxane	36	376	431	3393.8	0.0245
DMF	43.2	378	473	5313.4	0.2743
DMSO	45.1	380	481	5525.8	0.2637
Hexane	31	369	389	1393.3	0.0137
Methanol	55.4	376	432	3447.6	0.3085
i-PrOH	48.4	377	459	4738.7	0.2721
Nitromethane	46.3	377	425	2995.7	0.290
THF	37.4	374	434	3696.5	0.2095