Supporting information

A fluorescent organic cage for picric acid detection

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Experimental section:

Materials and methods: All chemicals and solvents were purchased from commercially available sources and were used without further purification.1,3,5-tris(aminomethyl)-2,4,6-trimethylbenzene[1] (**2**) was synthesized according to the reported procedure.^{1}H, ^{13}C NMR spectra for the characterization of the products were recorded on a Bruker 400 MHz spectrometer. In ^{1}H NMR spectra chemical shift (δ) values are enlisted in ppm relative to the TMS (0.00 ppm) as an internal standard in $CDCl_3$. Bruker ALPHA FTIR spectrometer was used for recording IR spectra. High resolution mass spectra wererecorded on a Q-TOF instrument by electrospray ionization (ESI) technique.Electronic absorption and emission spectra were recorded using a Perkin-Elmer LAMBDA 750 UV-visible spectrophotometer and a HORIBA JOBIN YVON made Fluoromax-4 spectrometer, respectively. All solvents used were of standardspectroscopic grade. Solution state quantum yield was estimated by comparing with quinine sulphate (Φ= 0.57 in 0.1 M H_2SO_4).Solid state quantum yield was obtained using "Integrated Sphere" coupled with a HORIBA JOBIN YVON made Fluoromax-4 spectrometer.

Cage 3: In a 250 mL round bottom flask 120 mL $CHCl_3$ solution of triamine**2** (92 mg, 0.44 mmol)was added slowly drop-wise to a stirring solution of aldehyde **1** (200 mg, 0.66 mmol)

dissolved in 60 mL $CHCl_3$. Resulting reaction mixture was heated to reflux for 24h. After completion of the reaction, solvent was completely removed and the obtained pale yellow solid was washed with acetonitrile to remove unreacted staring materials. Isolated yield: 85 % (226 mg, 0.19mmol).

^{1}H NMR ($CDCl_3$, 400MHz): δ 2.36 (s, 18H), 4.90 (s, 12H), 7.03 (d, 12H), 7.12 (m, 9H), 7.30 (t, 6H), 7.56 (d, 12H), 8.16 (s, 6H) ; ^{13}C NMR (100 MHz, $CDCl_3$): δ 16.6, 59.0, 123.4, 124.9, 126.6, 129.6, 130.0, 131.4, 133.6, 137.6, 147.2, 149.7, 160.2. FTIR (cm^{-1}) ν: 2862, 2029, 1635 (CH=N), 1594, 1503,1306, 1271, 1165, 821, 751, 690, 518.

Cage 4: In a 250 mL round bottom flask, 180 mg (0.15mmol) of cage **3** was taken in $CHCl_3$-MeOH (1:1, v/v) binary solvent mixture. Into above reaction mixture,68 mg (1.8 mmol) of $NaBH_4$ was added at room temperature and stirred for 1h followed by reflux for 12h.After completion of the reaction, solvent was completely removed and the product was extracted in $CHCl_3$.Organic part was washed with water for 3 to 4 times and dried over sodium sulphate followed by removal of solvent to get white solid. Isolated yield: 92% (169 mg, 0.14mmol).

^{1}H NMR ($CDCl_3$, 400MHz): δ 1.44 (br, 6H), 2.50 (s, 18H), 3.85 (s, 12H), 3.90 (s, 12H), 6.96-6.98 (m, 15H), 7.05 (d, 6H), 7.18-7.24 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): 16.2, 49.8, 54.8, 122.8, 124.5(124.49 and 124.46), 129.1, 129.6, 135.1, 135.3, 136.0, 147.0, 148.6; ESI-HRMS ($CHCl_3$/CH_3CN, 1:5), m/z $[M+H]^+$ 1222.7124 (calculated 1222.7162),$[M+2H]^{2+}$611.8612(calculated 611.8620). FTIR (cm^{-1}) ν: 2912, 2847, 1584, 1498, 1443, 1311, 1256, 1175, 1094, 1018, 801, 746, 685, 609.

Fluorescence quenching titration study: In a 1 cm quartz cuvette 2 mL solution of cage **4** in DCM was placed, which was titrated with 1×10^{-3} M DCM solution of PA. For each addition, at

least three fluorescence spectra were recorded repeatedly at ambient temperature to obtain concordant values. Cage**4** was excited at 304 nm and the emission spectra wererecordedin the region of 340-550 nm, while keeping 3 nm slit width for both source and detector.In presence of othernitroanalytes fluorescence intensitiesof the cage (2mL, 1×10^{-5} M)were recorded before and after addition of 2 eq. (40 μL, 1×10^{-3}M)analytes.

Fluorescence quenching efficiencieswere calculated by the following equation,

$$\eta = (I_0\text{-}I)/I_0 \times 100\%.$$

where, I_0andI are the intensities of the cage solution before and after addition of 2 eq. of analytes respectively. Quenching constants (K) was calculated from I_0/I vs [PA] plot by fitting the equation,

$$I_0/I = Ae^{K[PA]} + B.$$

Competitive experiment between PA with other nitroaromatics:

To a 1×10^{-5} M solution of cage,one eq. of each nitroaroamtic (except PA) was added initially which showed ~ 30 % quenching of fluorescence intensity. To the resulting solution mixture when only one eq. PA was added, dramatic change in fluorescence intensity was observed (quenching of initial fluorescence intensity ~ 80%), which further suggests higher sensitivity of the cage towards PA (Fig. S28).

Determination of cage - PA binding stoichiometry: Excess PA was added to a chloroform solution of cage **4.** Yellow ppt was formed in a few minutes. The resulting precipitate was filtered and washed several times with chloroform to remove unreacted PA and then ^{1}H NMR was checked in CD_3CN which suggested 1: 6 (cage : PA) complex formation.

X-ray Crystal Data Collection and Structure Solution: X-ray data of the cage**4**were collected on a BrukerSMART APEX CCD diffractometer using the SMART/SAINT software,[2]equipped with a low temperature device. Diffraction quality crystal was mounted on a loop coated with traces of paraton oil. The intensity data of cage **4** were collected at 100(2) K by using graphite monochromatic Mo-Kα radiation (0.7107 Å). The structure wassolved by direct method and refined by full-matrixleast squares on F^2, employing the SHELX-97[3]incorporated in WinGX.[4] Empirical absorption corrections were applied with SADABS.[5] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were assigned by using the riding models and refined isotropically. Crystallographic data and refinement parameters are provided inTable S1. Disordered solvent molecules were treated using the SQUEEZEprogram in PLATON.[6]

Computational Methodology: Full geometry optimizations were carried out using Gaussian 09 package.[7]The hybrid B3LYP functional has been used in all calculations as implemented in *Gaussian 09* package, mixing the exact Hartree-Fock-type exchange with Becke's expression for the exchange functional[8] and that proposed by Lee-Yang-Parr for the correlation contribution.[9] The 6-31G basis set was used for all calculations. Frequency calculations carried on the optimized structures confirmed the absence of any imaginary frequencies.

Table S1. Crystallographic data and refinement parameters for cage **4**.

	Cage 4
Empirical formula	$C_{84}H_{87}N_9$
Fw	1222.63
T (K)	100(2)
crystal system	Monoclinic
space group	C *2/c*
a/Å	26.9032(15)
b/Å	16.3699(8)

c/Å	19.1527(10)
α/deg	90.00
β/deg	90.698(3)
γ/deg	90.00
V/Å^3	8434.3(8)
Z	4
*ρ*calcd (g cm^{-3})	0.963
μ(Mo K) (mm^{-1})	0.057
λ/Å	0.71073
F (000)	2616.0
unique reflns	7392
GOF *(F²)*	1.037
$R_1{}^a$	0.0772
$wR_2{}^b$	0.2331

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR_2 = [\Sigma\{w(F_o^2 - F_c^2)^2\}/\Sigma\{w(F_o^2)^2\}]^{1/2}$

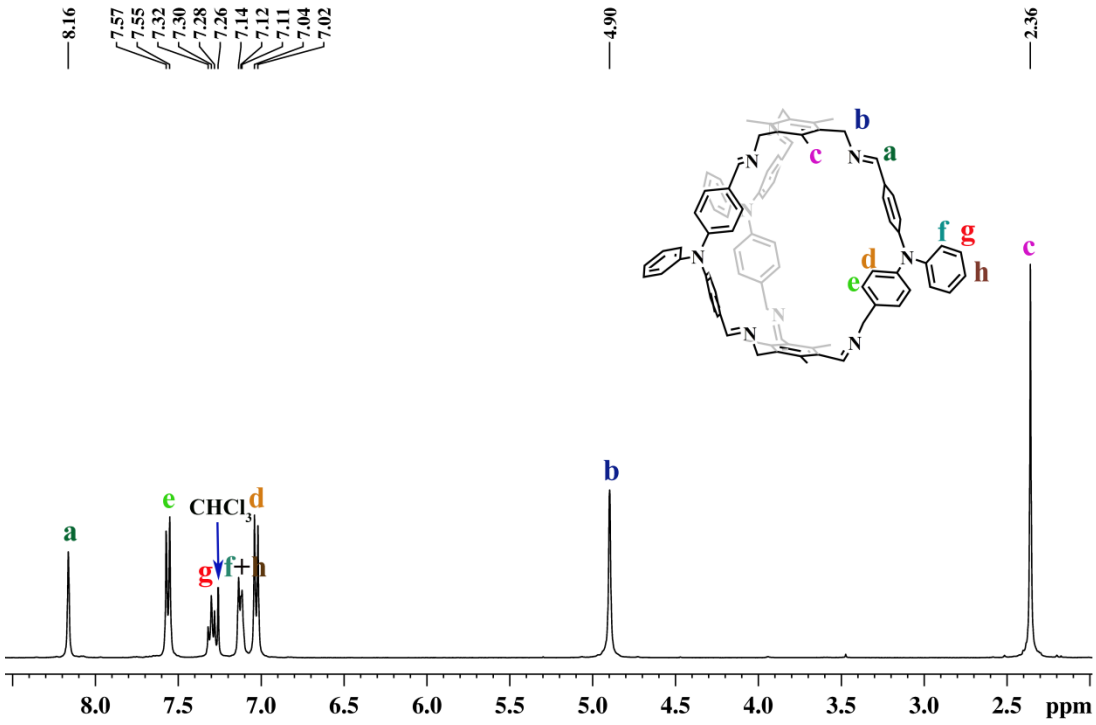

Fig. S1: ^{1}H NMR spectrum of cage **3** recorded in $CDCl_3$.

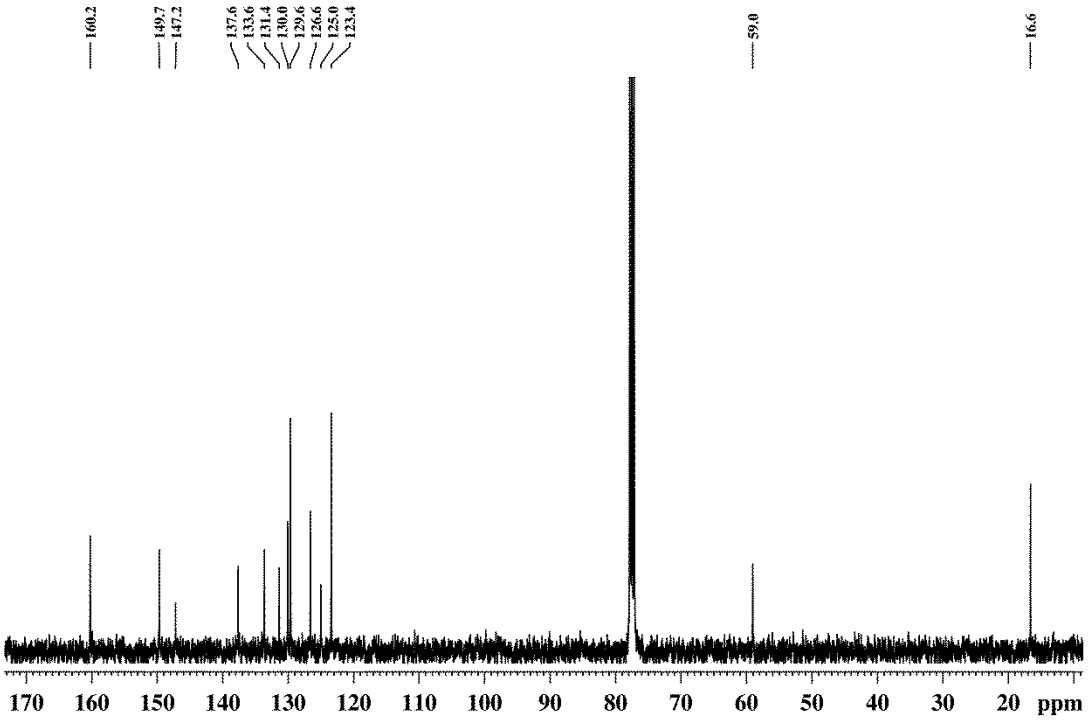

Fig. S2: ^{13}C NMR spectrum of cage **3** recorded in $CDCl_3$.

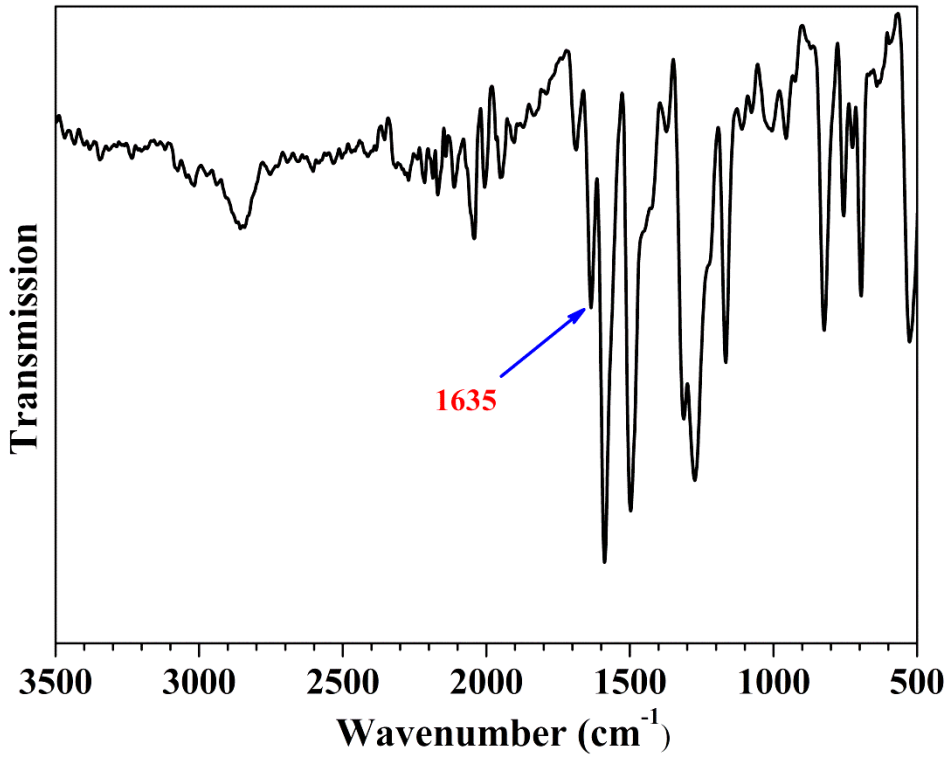

Fig. S3: FTIR spectrum of cage **3**.

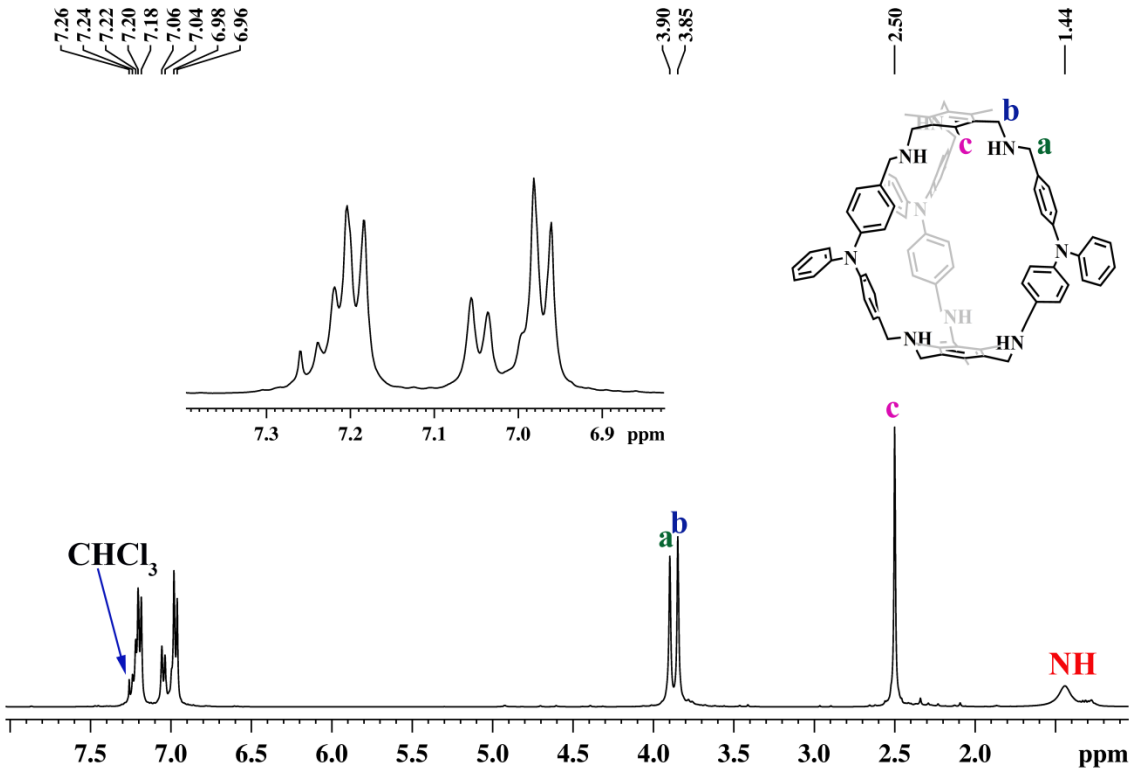

Fig. S4: ^{1}H NMR spectrum of cage **4** recorded in $CDCl_3$.

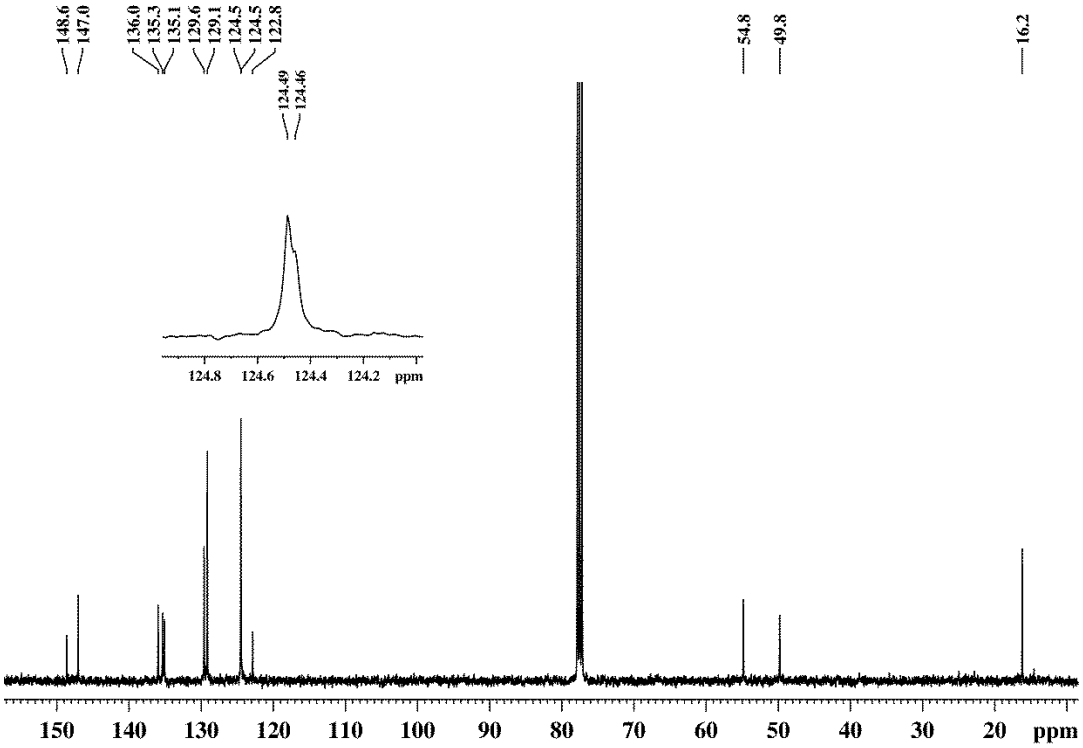

Fig. S5: ^{13}C NMR spectrum of cage **4** recorded in $CDCl_3$.

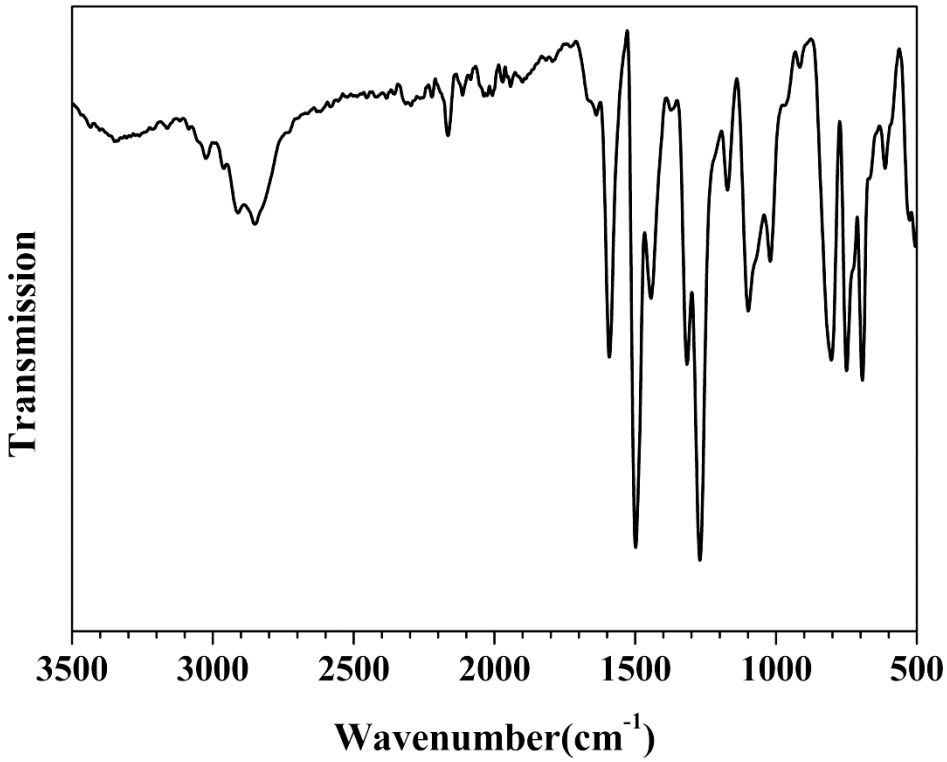

Fig. S6: FTIR spectrum of cage **4**.

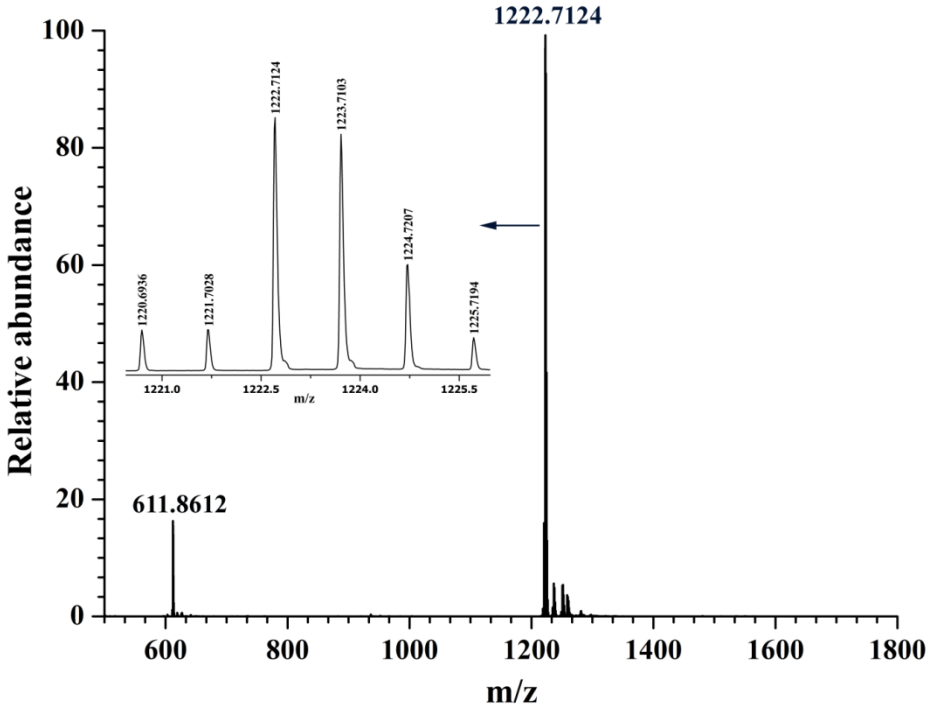

Fig. S7: ESI-HRMS spectrum of cage **4** recorded in $CHCl_3$-MeCN (1:5, v/v).

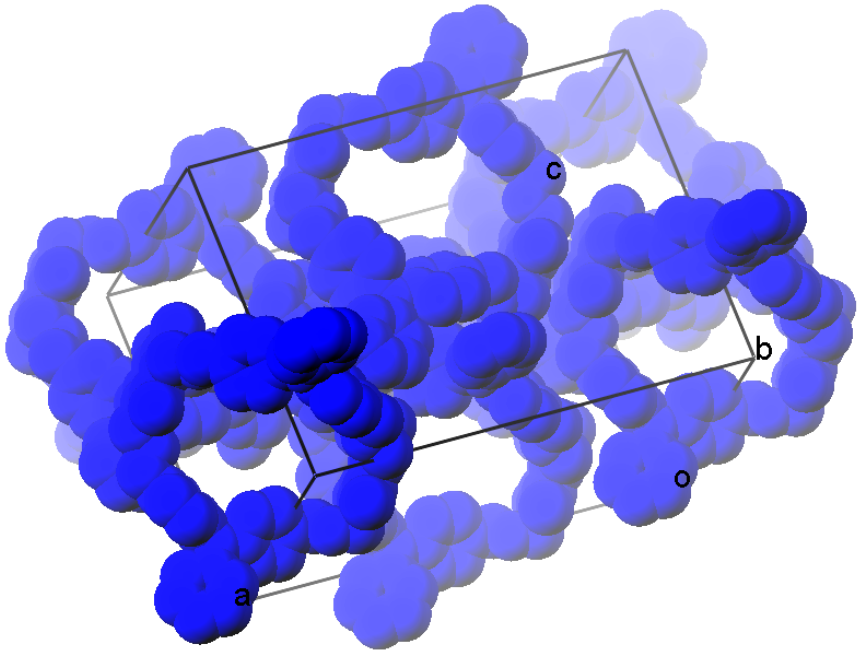

Fig. S8: Unit cell packing diagram of cage **4**. Hydrogen atoms are omitted for clarity.

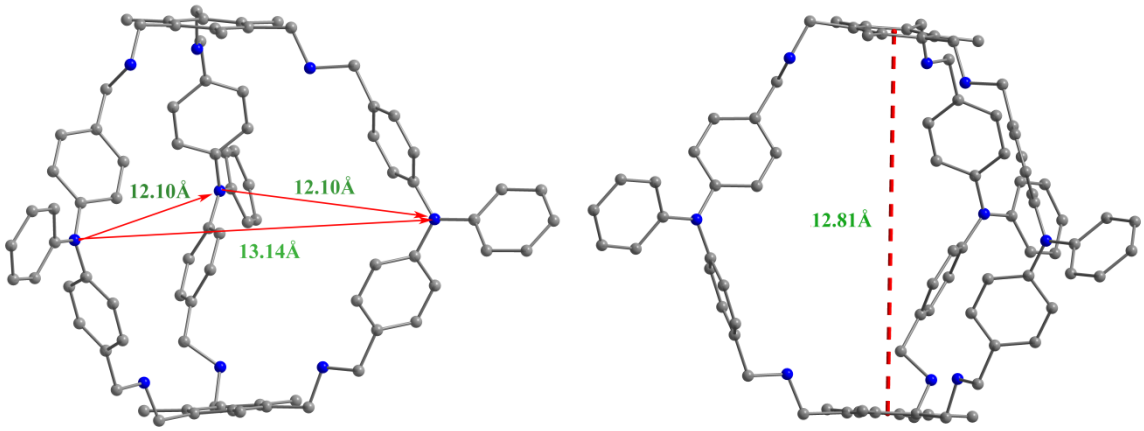

Fig.S9: Molecular dimensions of cage **4** obtained from single crystal structure analysis.

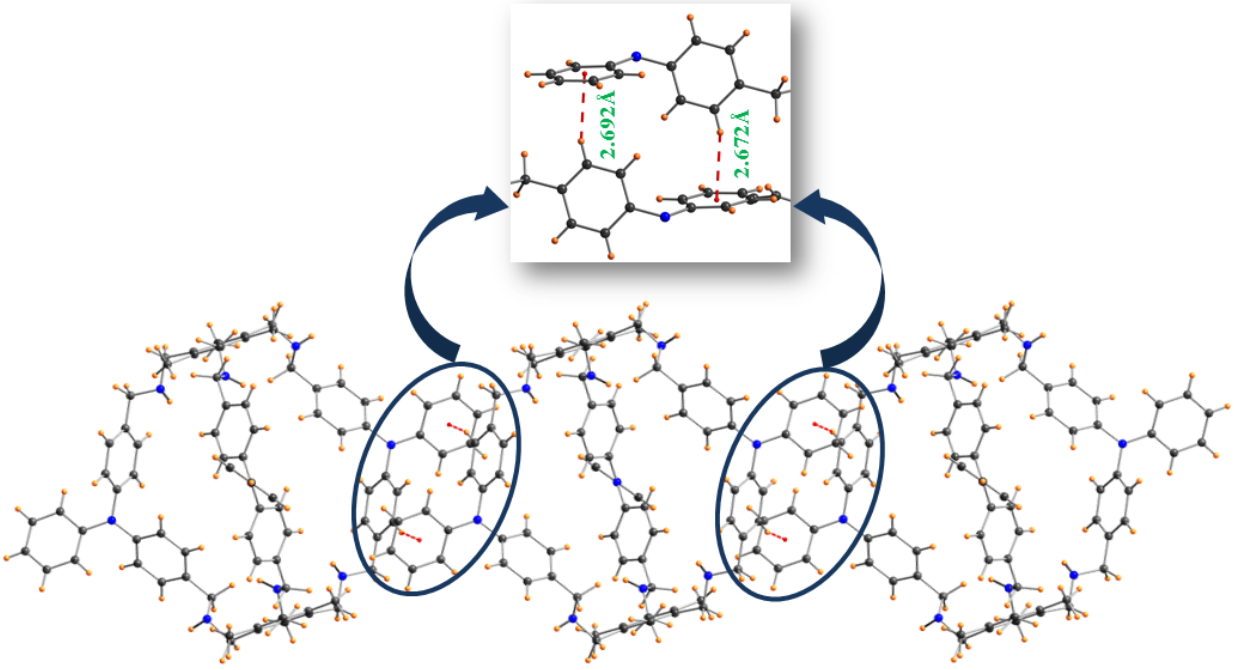

Fig.S10:1D supramolecular chain of cage **4***via* C-H…π interaction.

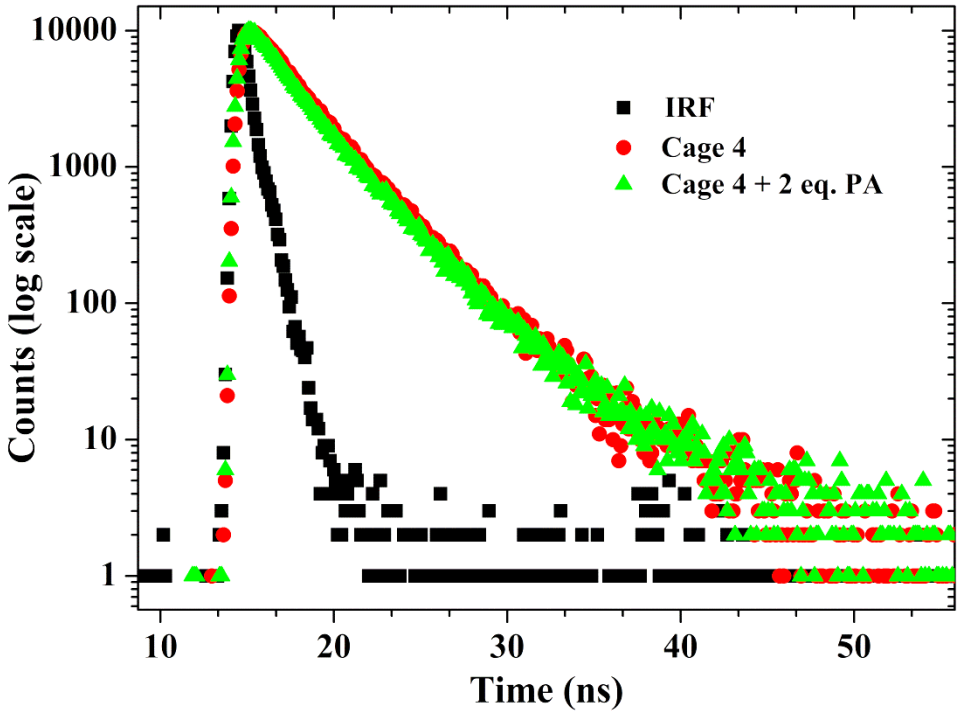

Fig.S11: Lifetime decay profile of cage **4** (2 mL, 1×10^{-5}M) in presence of picric acid recorded in DCM, IRF= instrument response function. (λ_{ex} = 305 nm, monitored at 435 nm)

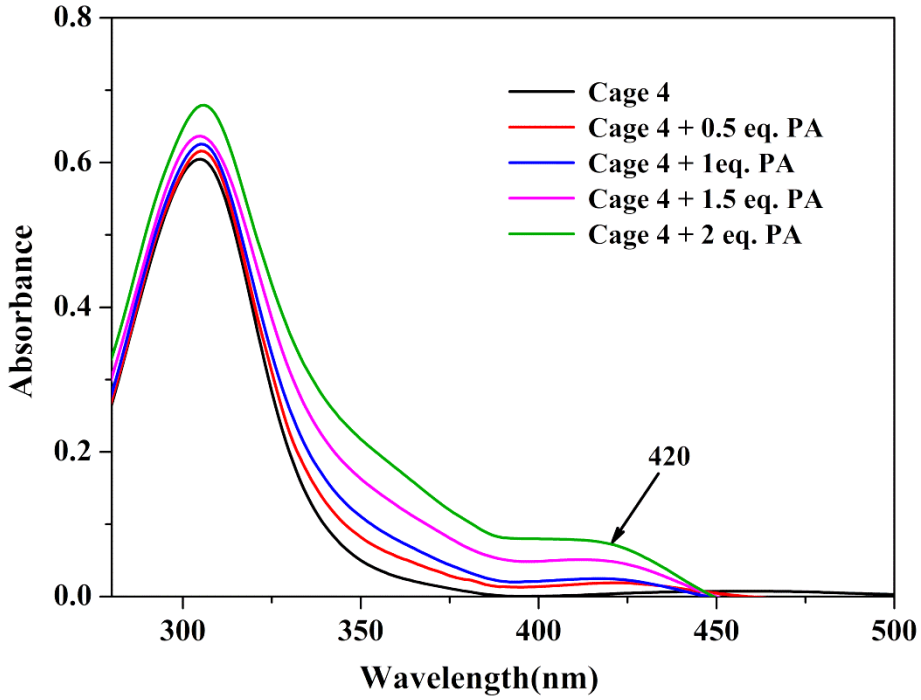

Fig.S12: UV-vis spectra of cage **4** upon gradual addition of PA in DCM, showing spectral change with the appearance of new band at 420 nm.

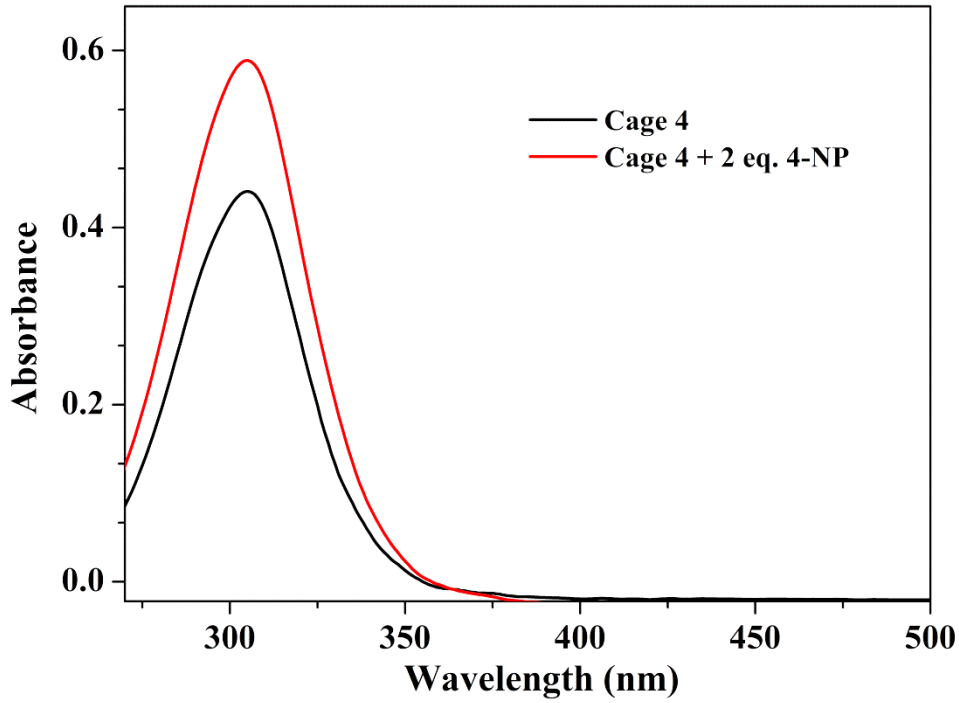

Fig.S13:UV-vis spectra of cage **4** before and after addition of 2 eq. of 4-NP.

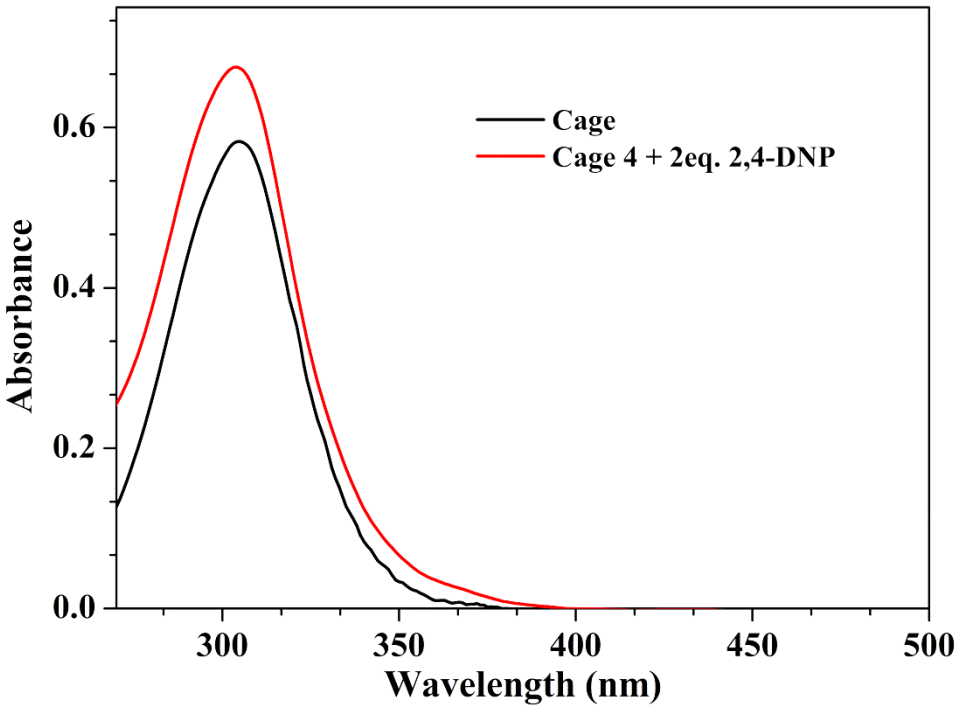

Fig.S14:UV-vis spectra of cage **4** before and after addition of 2 eq. of 2, 4-DNP.

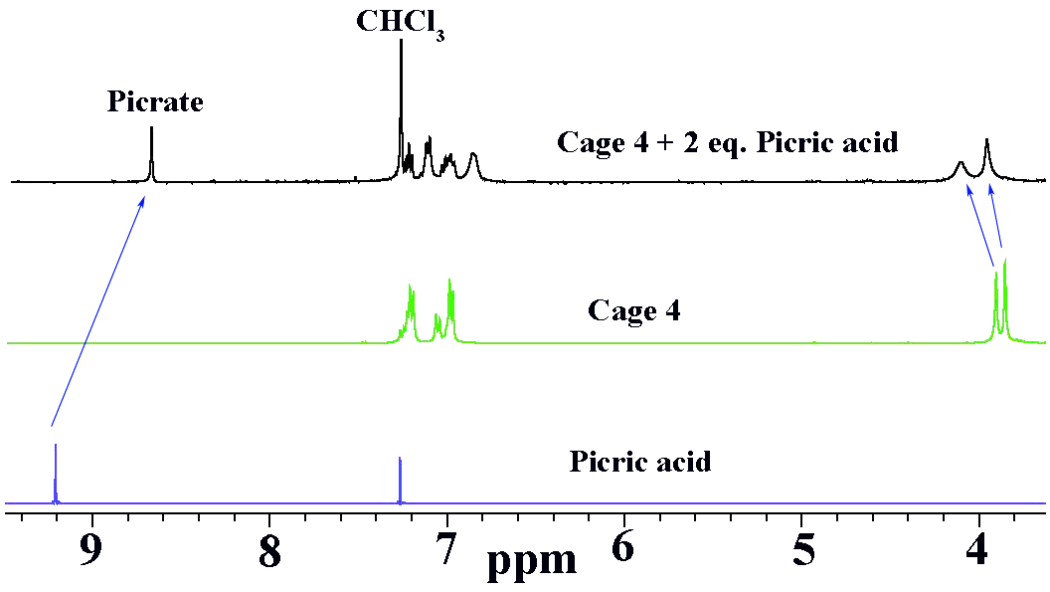

Fig.S15: ^{1}H NMR spectra of cage **4** before and after addition of 2 eq. of PA recorded in $CDCl_3$.

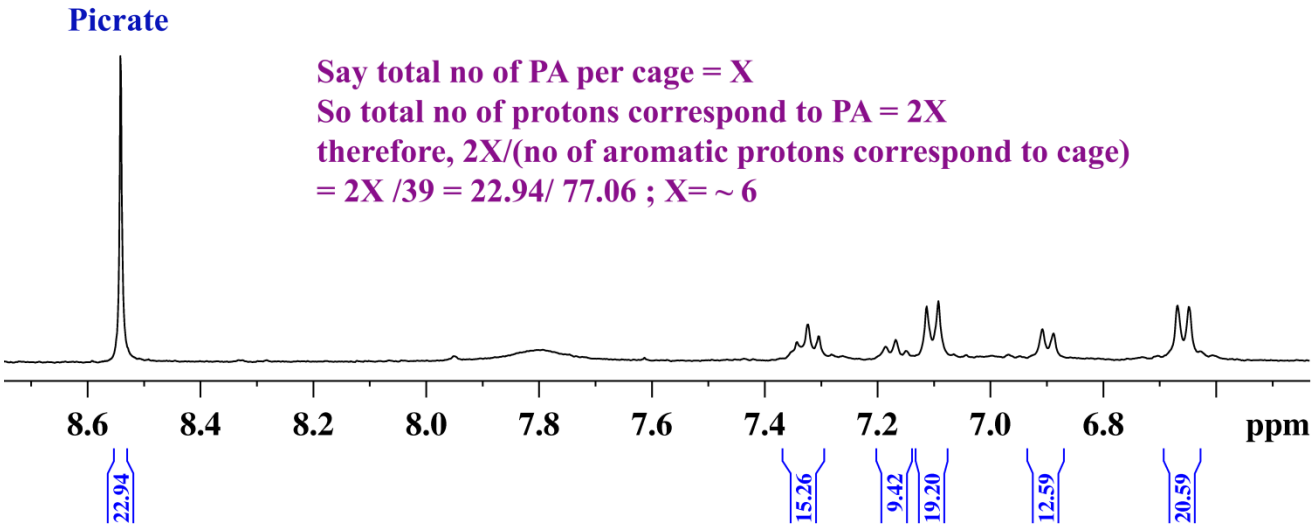

Fig. S16: Partial ^{1}H NMR spectrum of cage **4** - PA complex recorded in CD_3CN.

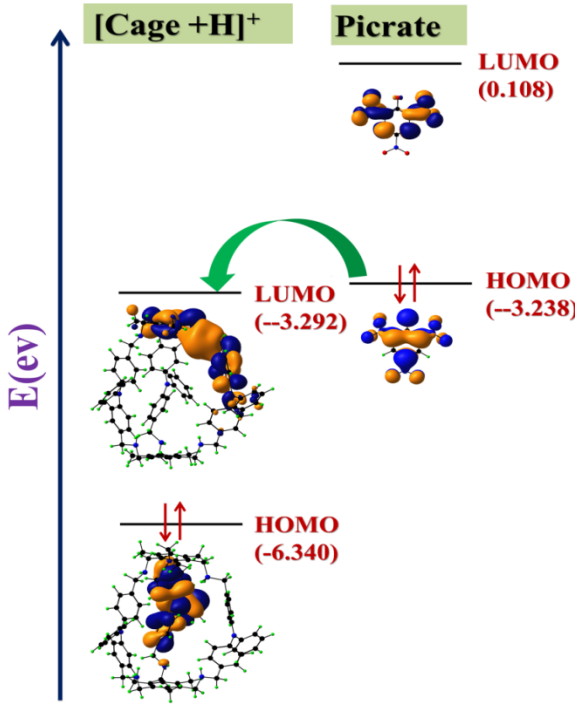

Fig.S17: Pictorial representation of ground state charge transfer process occurring from HOMO of the picrate anion to the LUMO of the protonated cage **4**.

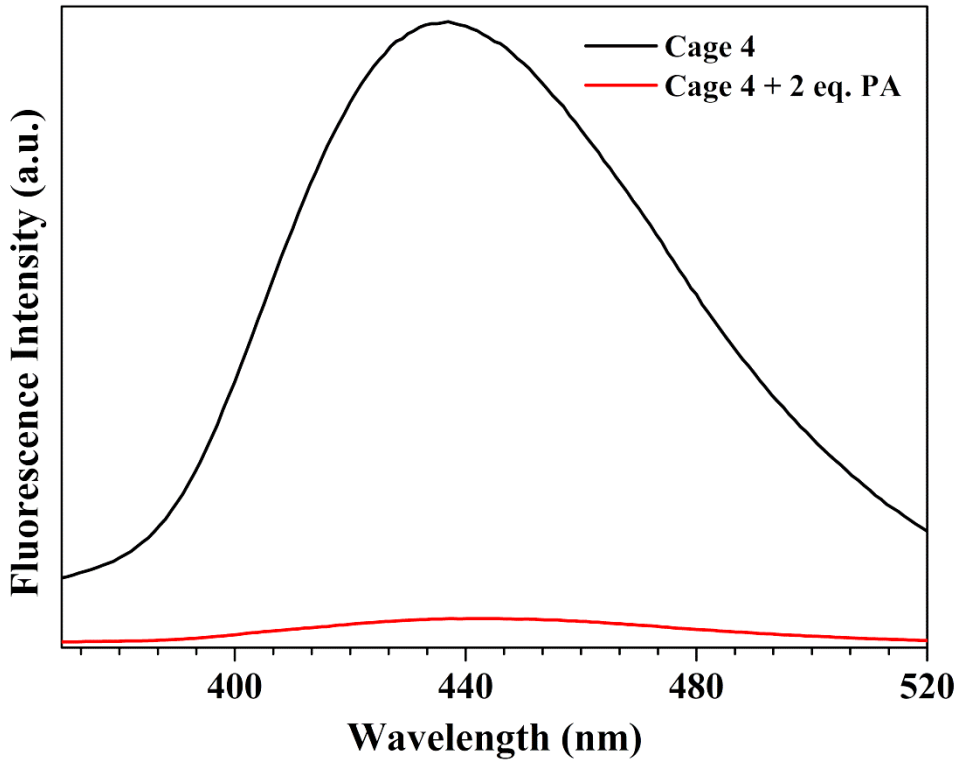

Fig.S18: Change in the fluorescence spectrum of cage **4** upon addition of 2 eq. of PA in DCM.

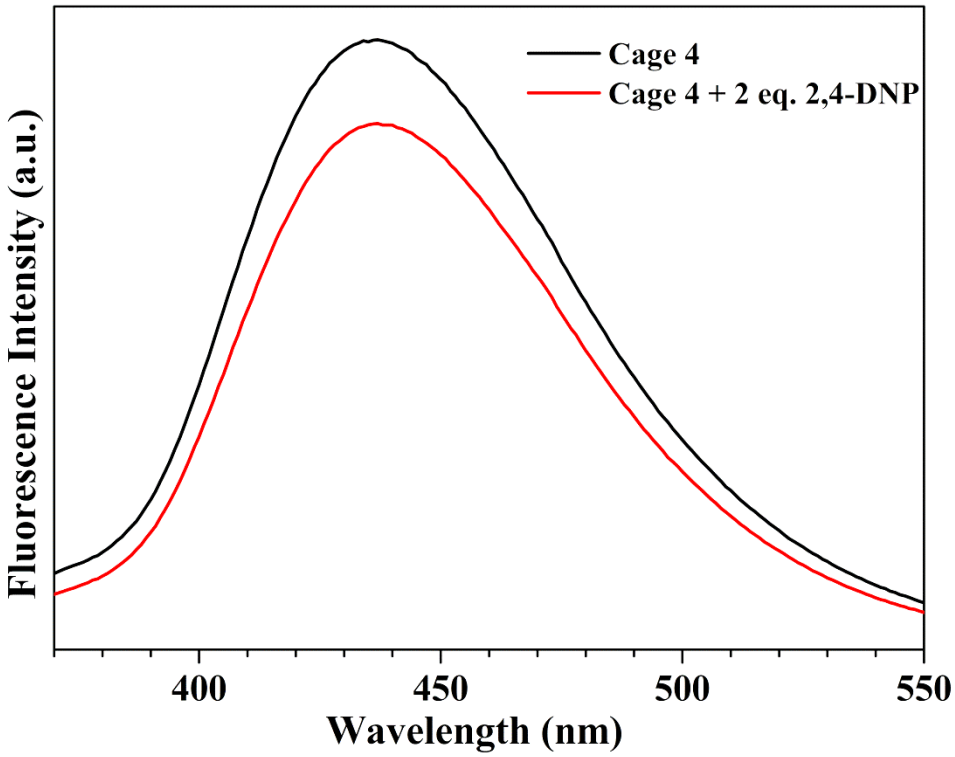

Fig.S19: Change in the fluorescence intensity of cage **4** upon addition of 2 eq. of 2, 4-DNP in DCM.

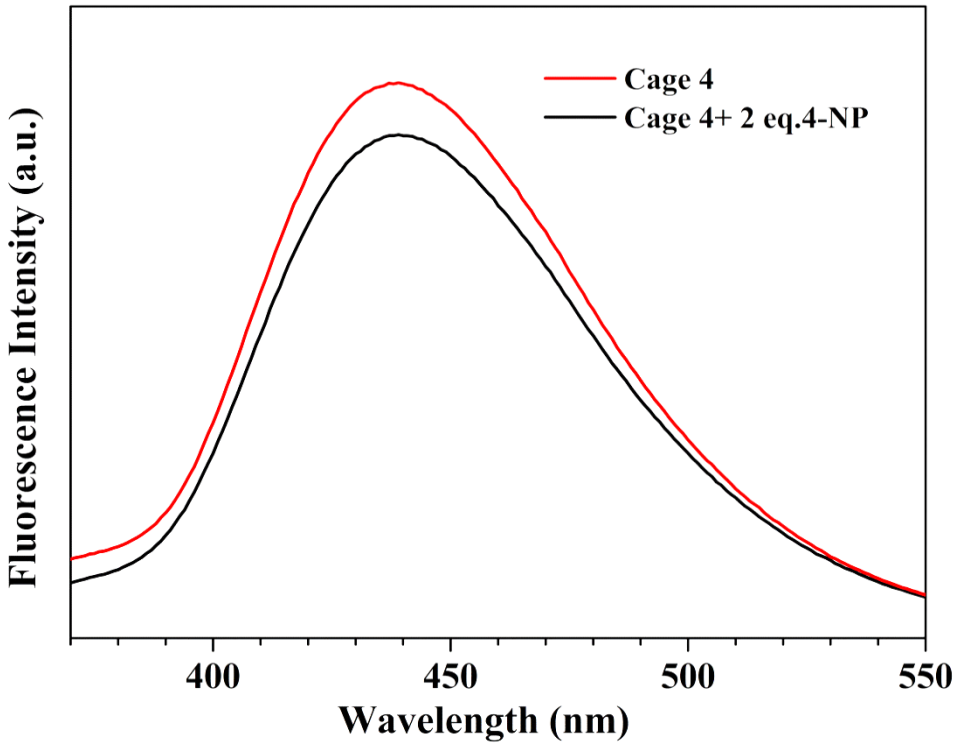

Fig.S20: Change in the fluorescence intensity of cage **4** upon addition of 2 eq. of 4-NP in DCM.

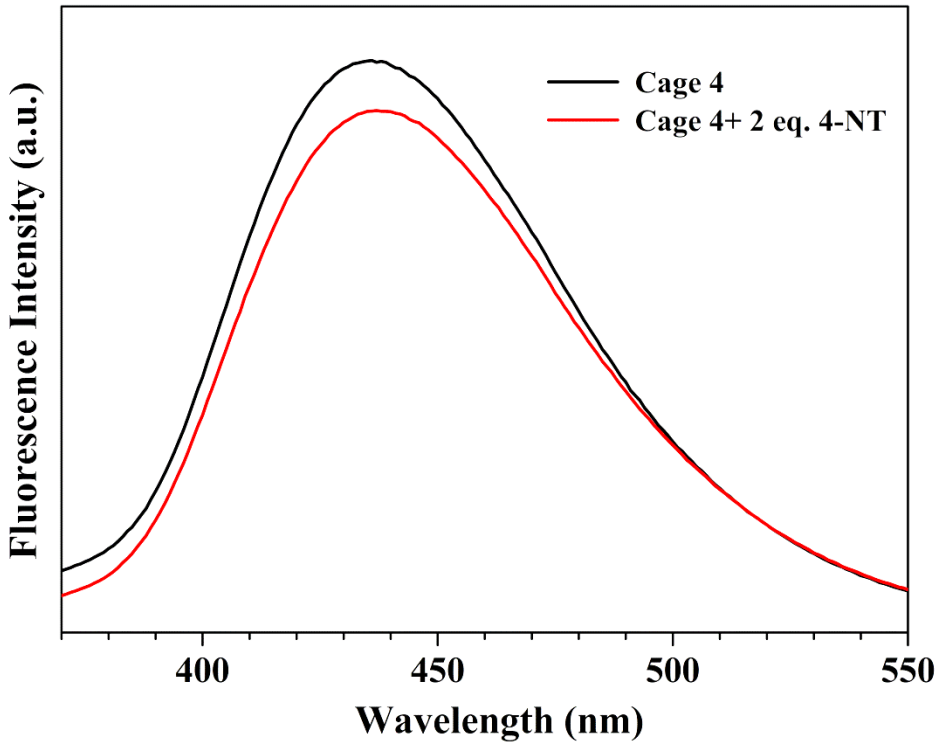

Fig.S21: Change in the fluorescence intensity of cage **4** with the addition of 2 eq. of 4-NT in DCM.

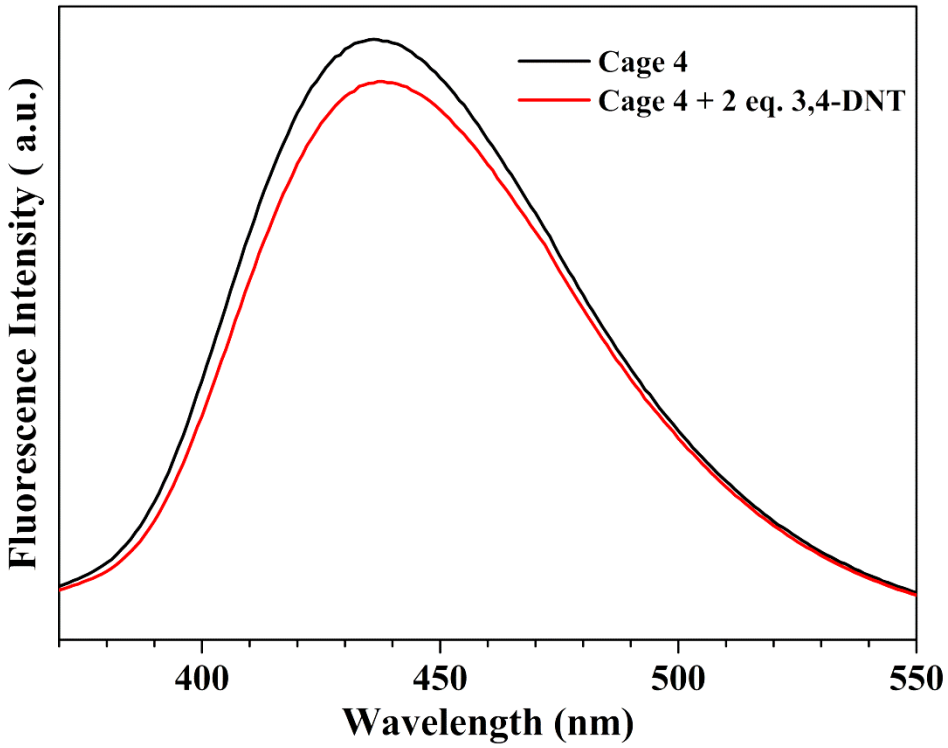

Fig.S22: Change in the fluorescence intensity of cage **4** upon addition of 2 eq. of 3, 4-DNT in DCM.

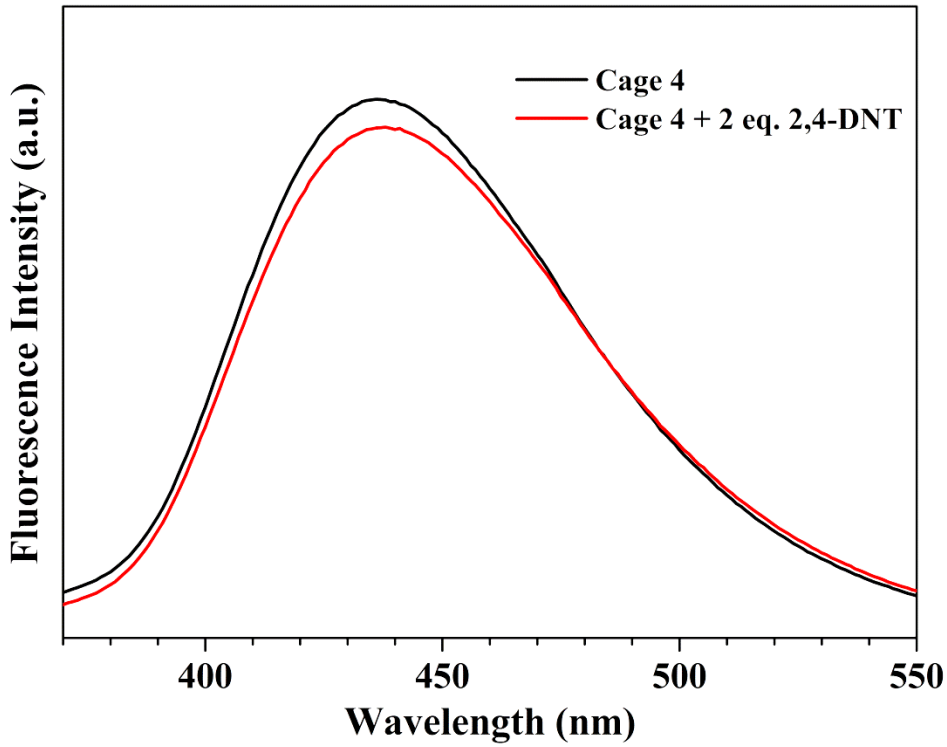

Fig.S23: Change in the fluorescence intensity of cage **4** upon addition of 2 eq. of 2, 4-DNT in DCM.

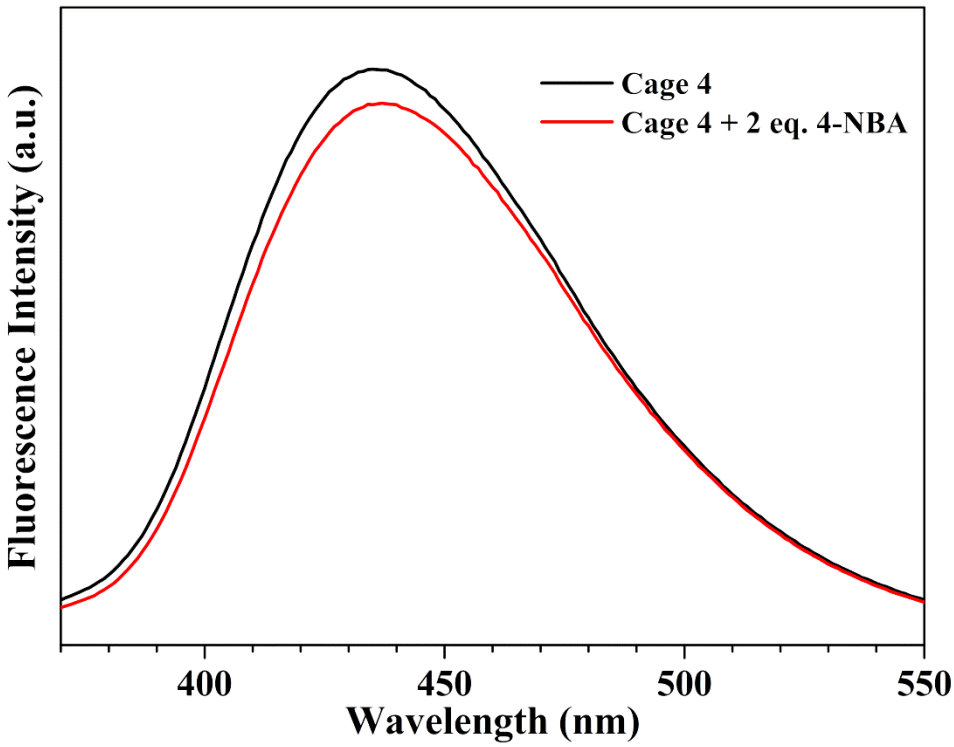

Fig.S24: Change in the fluorescence intensity of cage **4** upon addition of 2 eq. of 4-NBA in DCM.

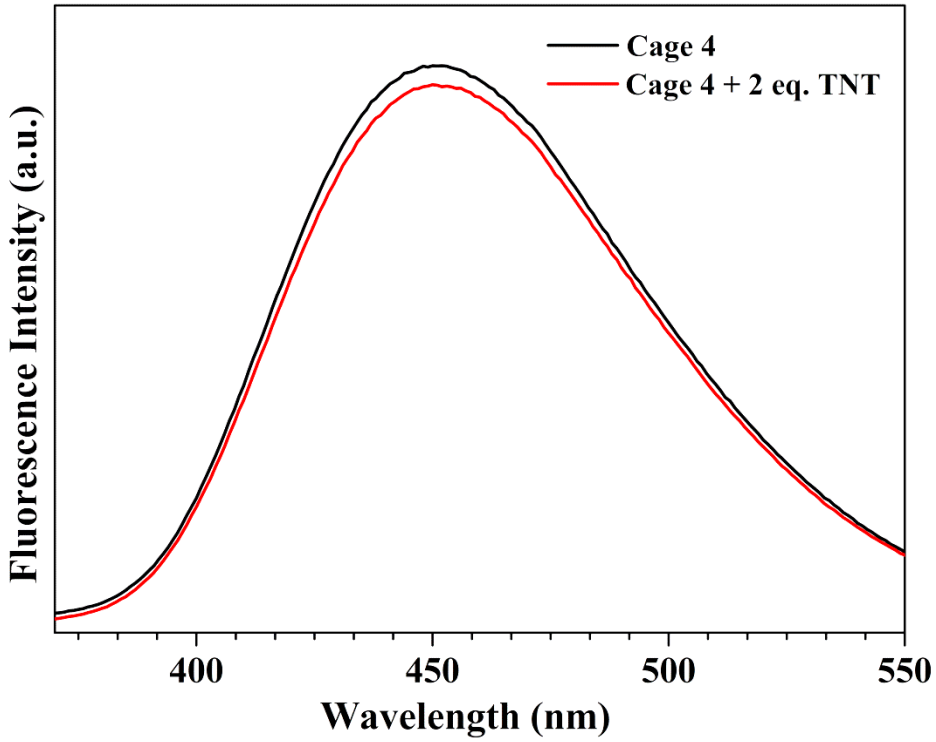

Fig.S25: Change in the fluorescence intensity of cage **4** upon addition of 2 eq. of TNT in DCM.

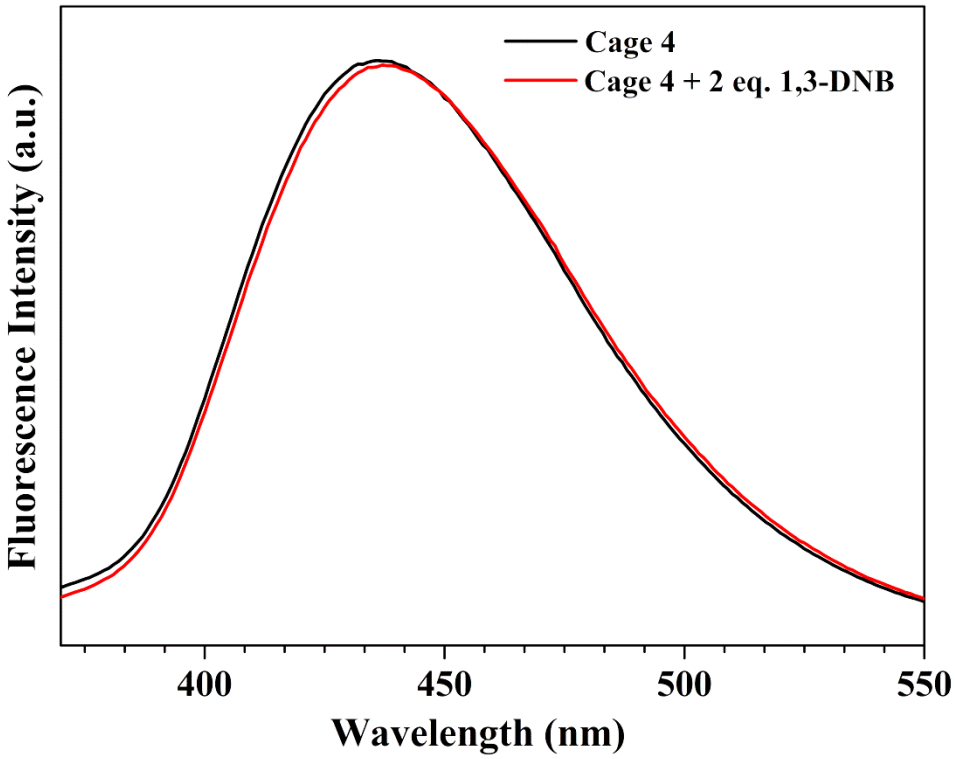

Fig.S26: Change in the fluorescence intensity of cage **4** upon addition of 2 eq. of 1, 3-DNB in DCM.

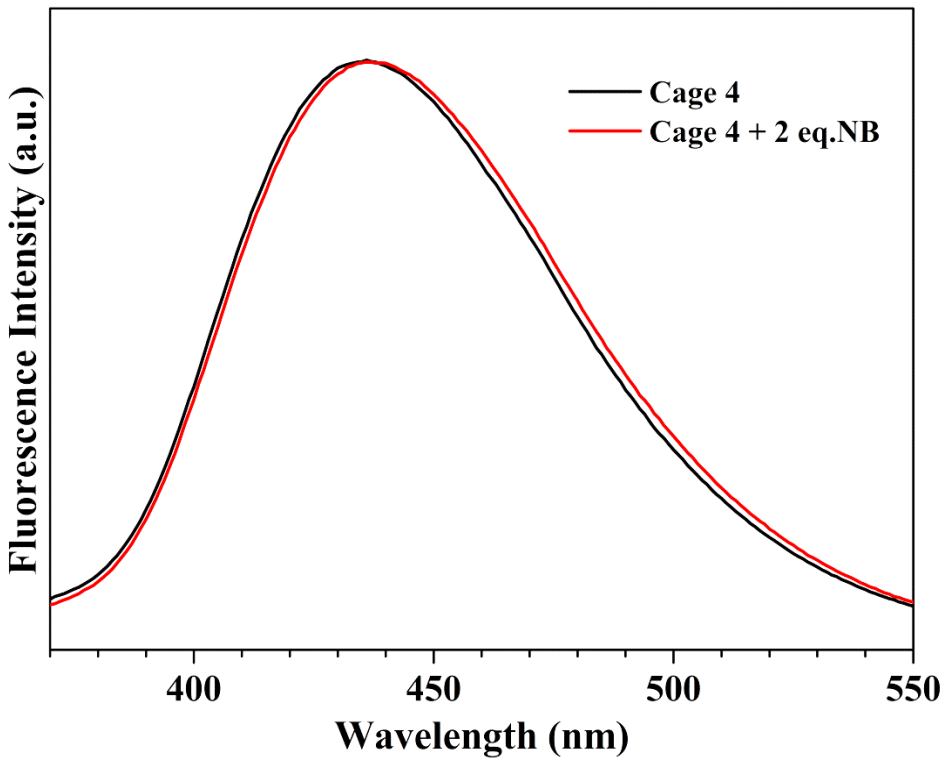

Fig.S27: Change in the fluorescence intensity of cage **4**upon addition of 2 eq. of NB in DCM.

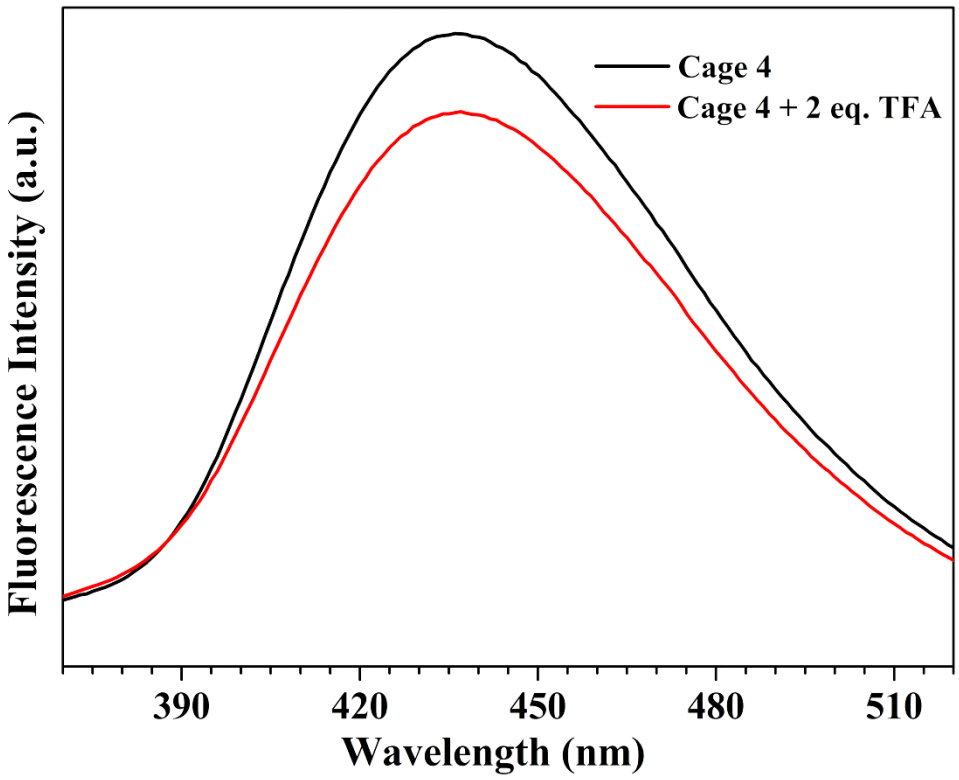

Fig.S28: Change in the fluorescence intensity of cage **4** upon addition of 2 eq. of TFA in DCM.

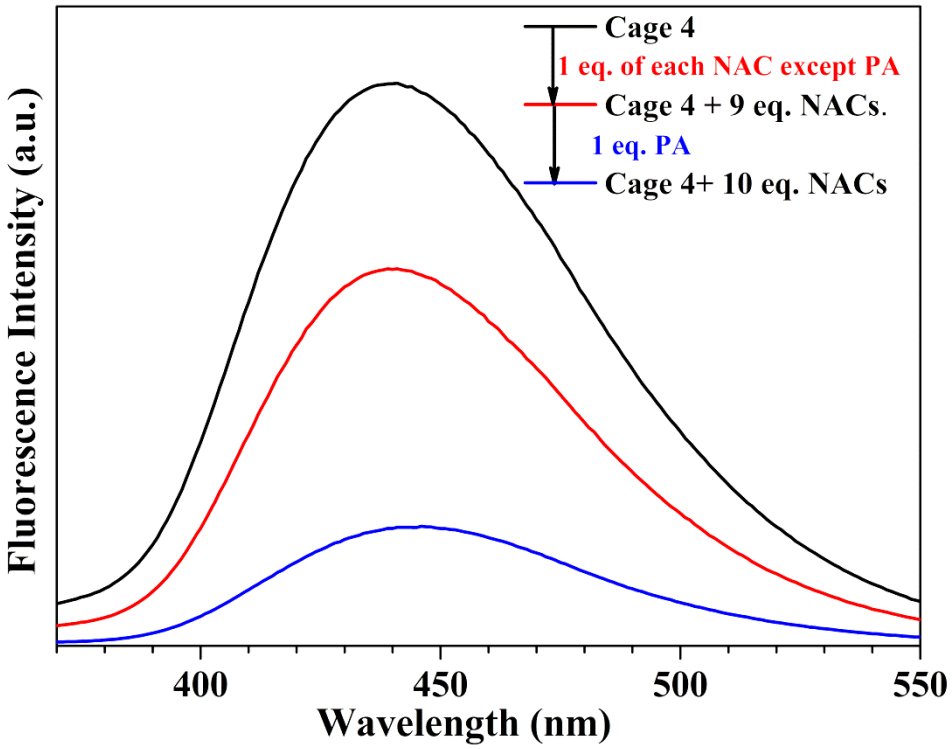

Fig.S29: Change in the fluorescence intensity of cage **4** upon the step wise addition of NACs.

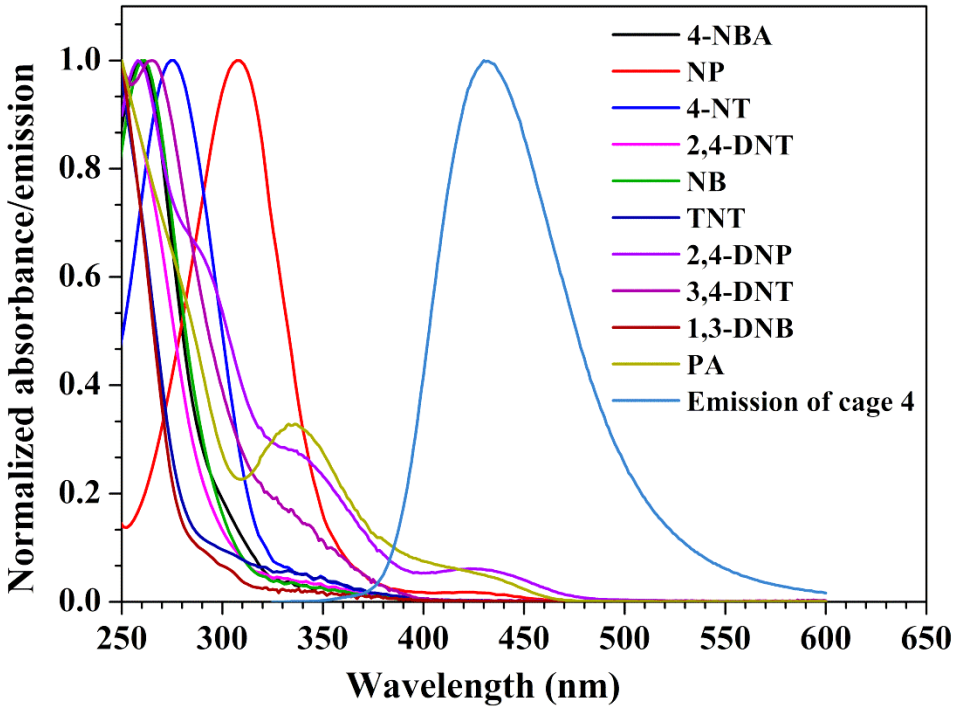

Fig.S30: Spectral overlap between normalized absorption spectra of nitro analytes and emission spectra of cage **4** in DCM.

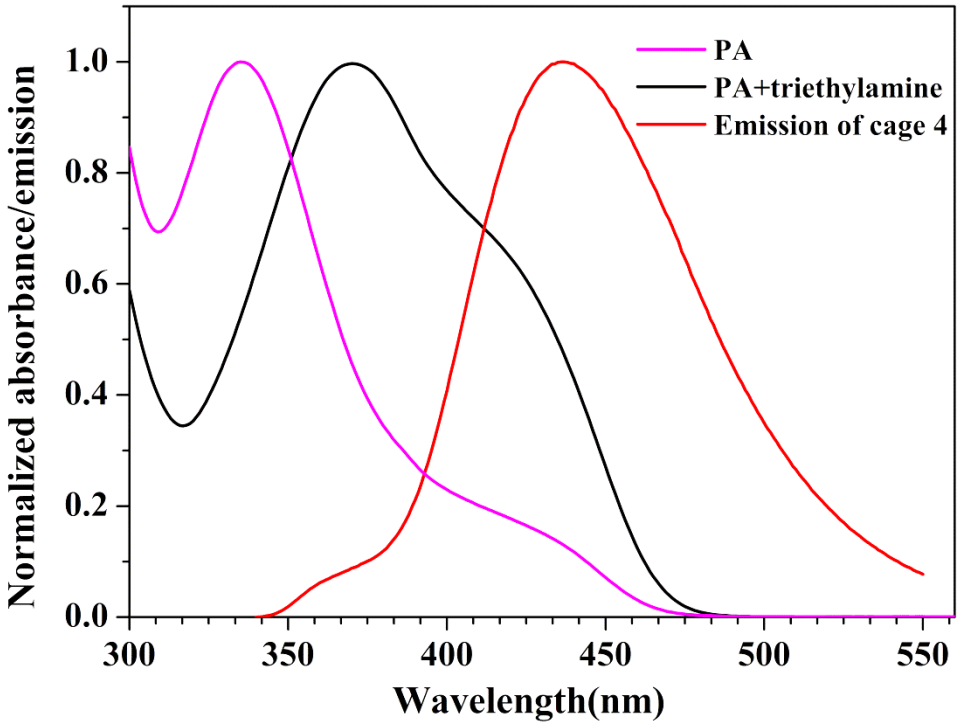

Fig.S31: Spectral overlap between normalized absorption spectra of picric acid, picric acid in presence of triethylamine and emission spectra of cage **4**in DCM.

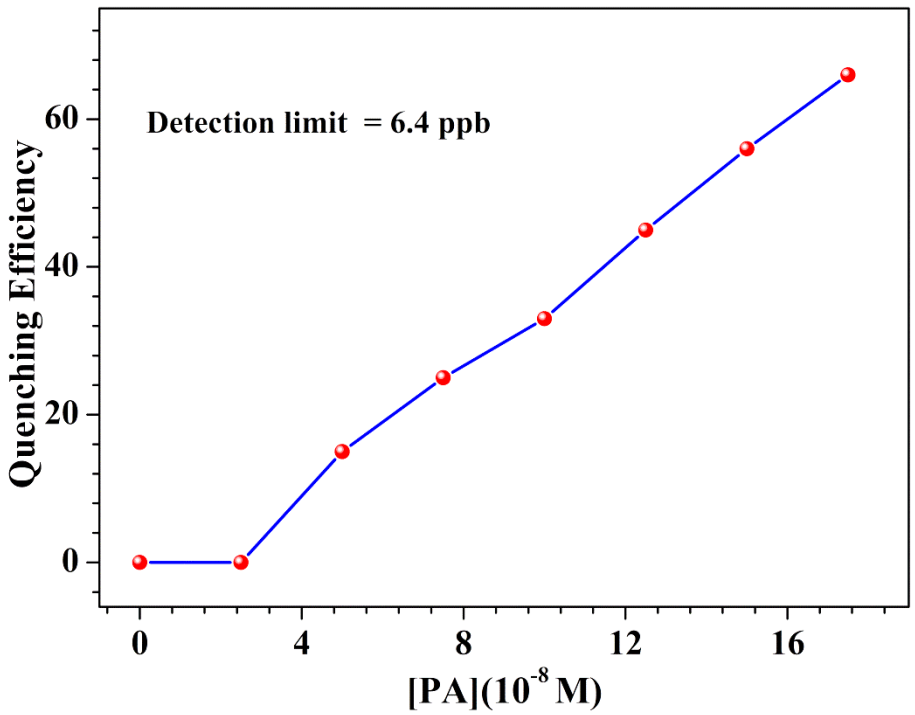

Fig.32: The plot of quenching efficiency *versus* amount of picric acid used for 10^{-6} M solution of cage in DCM. Detection limit was calculated using the formula, [PA] × MW_{PA} ×10^6.

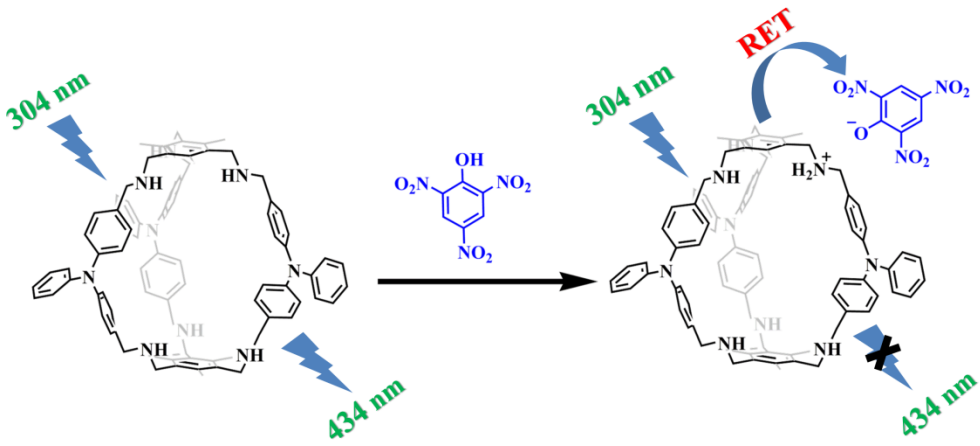

Fig.S33: Schematic diagram of fluorescence quenching by resonance energy transfer (RET) process.

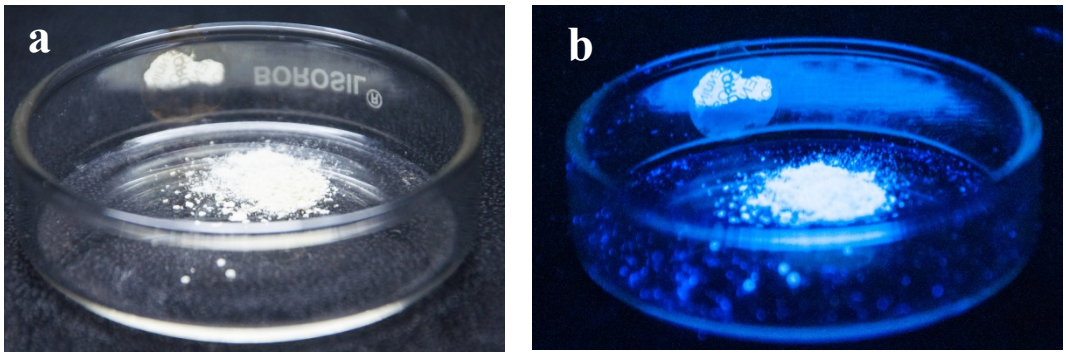

Fig.34: Digital photographs of the solid cage **4** under (a) normal light and (b) portable UV light.

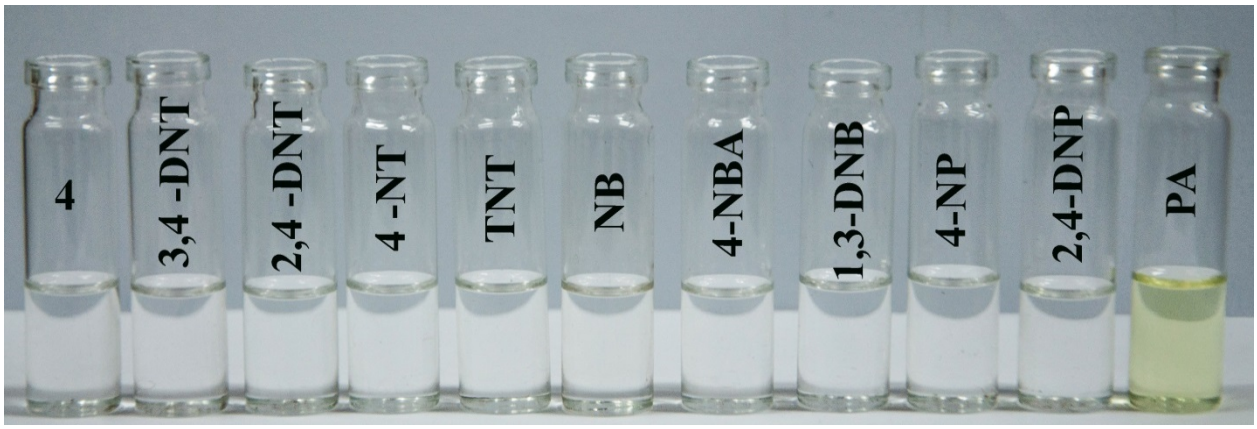

Fig.S35: Digital photograph of cage **4** solutions under normal light in presence of different nitroaromaticanalytes (2 eq.).

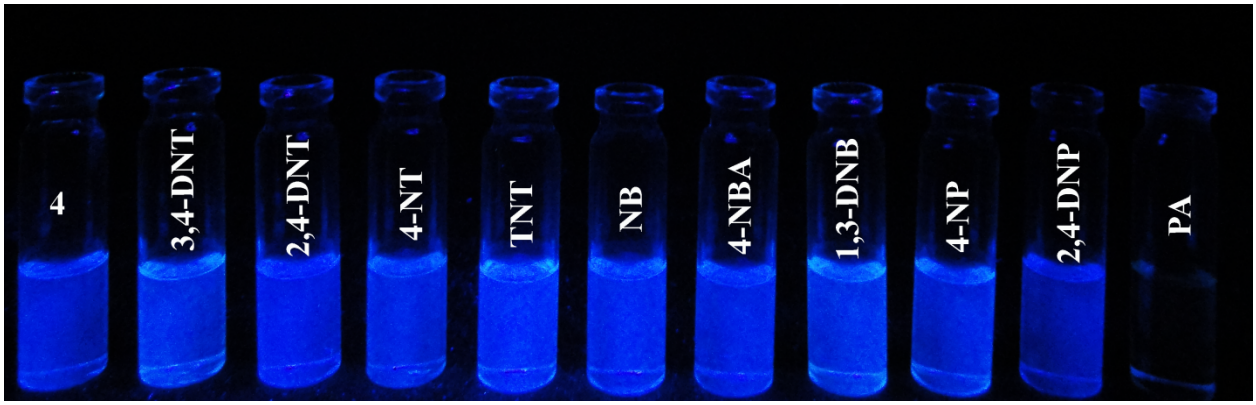

Fig.S36: Digital photograph of cage **4** solutions under portable UV light in presence of different nitroaromaticanalytes (2 eq.).

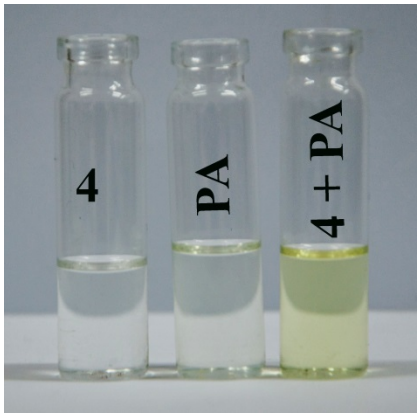

Fig.S37: Digital photograph of solutions of cage **4**, picric acid and cage in presence of picric acid in DCM, under normal light.

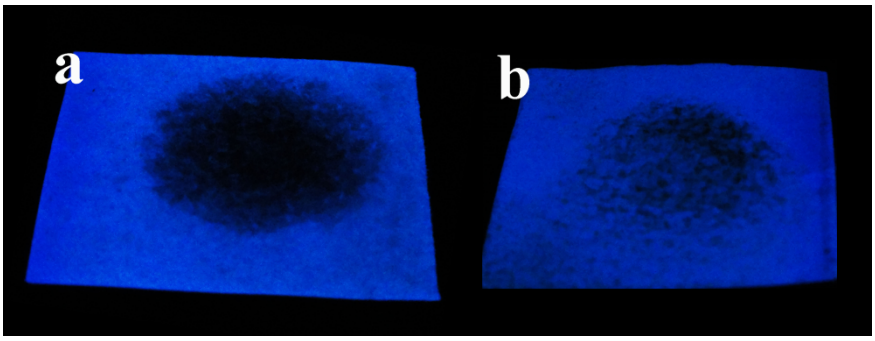

Fig.S38: Digital photograph of paper strips coated with cage **4** (a) after addition of 10µL (1mM) solution of picric acid and (b) after rubbing small amount of solid picric acid, under portable UV light.

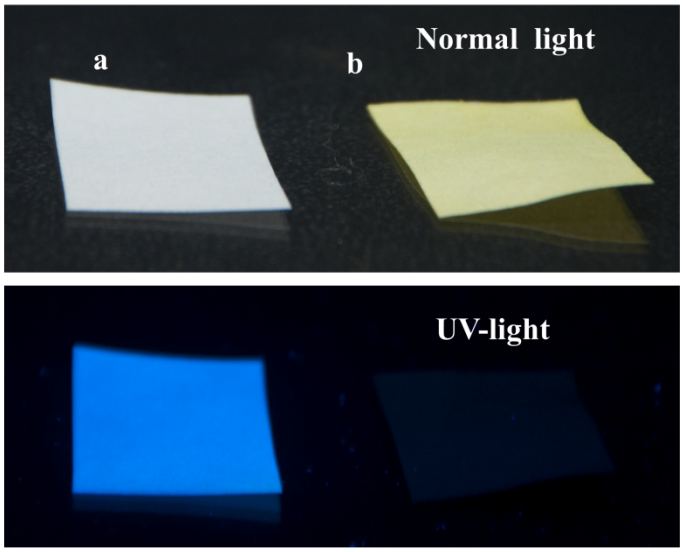

Fig. S39: Digital photographs of paper strips (placed over a glass slide) coated with cage **4** after dipping into (a) tap water and (b) tap water solution of picric acid, under normal light (top) and under portable UV light (bottom).

[Cage 4+H]$^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.579705	6.614971	0.604503
2	6	0	-0.195179	6.586890	0.870588
3	6	0	0.734543	6.555805	-0.194201
4	6	0	0.272938	6.626004	-1.524438
5	6	0	-1.116741	6.665485	-1.802361
6	6	0	-2.042764	6.677268	-0.734392
7	6	0	-2.595930	6.586455	1.734765
8	1	0	-2.179165	6.172508	2.655598
9	1	0	-3.449825	5.967532	1.447677
10	1	0	-2.971414	7.592293	1.974007
11	6	0	2.221985	6.450455	0.091873
12	1	0	2.730807	5.937194	-0.727099
13	1	0	2.398162	5.874470	1.003455
14	1	0	2.685592	7.439657	0.221090
15	6	0	-1.580325	6.698051	-3.252555
16	1	0	-2.609993	6.359877	-3.367339
17	1	0	-0.963526	6.047326	-3.879860
18	1	0	-1.521548	7.708013	-3.680833
19	6	0	-3.544039	6.815217	-0.973626
20	1	0	-3.943927	7.547358	-0.263708
21	1	0	-3.733946	7.233742	-1.973954
22	6	0	-4.204177	4.540538	-1.808437
23	1	0	-3.148395	4.264095	-1.907083
24	1	0	-4.526844	4.929482	-2.794506
25	6	0	-5.031130	3.322127	-1.461498
26	6	0	-4.494913	2.277882	-0.690185
27	1	0	-3.464361	2.342678	-0.353845
28	6	0	-5.270424	1.174265	-0.333706
29	1	0	-4.847472	0.377587	0.268587
30	6	0	-6.613981	1.088381	-0.742148
31	6	0	-7.159860	2.127726	-1.514148
32	1	0	-8.192669	2.065793	-1.838322
33	6	0	-6.373584	3.227999	-1.864150
34	1	0	-6.805455	4.016948	-2.474440
35	6	0	-8.712605	0.165149	0.190295
36	6	0	-8.933771	1.210266	1.106364
37	1	0	-8.108756	1.851721	1.395082
38	6	0	-10.207779	1.419350	1.640606
39	1	0	-10.363244	2.230272	2.345248
40	6	0	-11.274508	0.584935	1.285512
41	1	0	-12.261114	0.747121	1.706160
42	6	0	-11.054758	-0.459613	0.379191
43	1	0	-11.875050	-1.107991	0.087743
44	6	0	-9.788368	-0.666303	-0.173586
45	1	0	-9.629673	-1.465546	-0.888719
46	6	0	0.316423	6.615568	2.301397
47	1	0	1.256517	7.176193	2.345778
48	1	0	-0.391430	7.164656	2.943649

49	6	0	1.124830	5.192395	4.176864
50	1	0	0.392488	5.497346	4.950979
51	1	0	1.940051	5.929221	4.236209
52	6	0	1.679899	3.823857	4.534194
53	6	0	2.058135	2.905827	3.541880
54	1	0	1.922151	3.181354	2.502421
55	6	0	2.625648	1.675513	3.886481
56	1	0	2.933258	0.978640	3.113182
57	6	0	2.825812	1.344647	5.234643
58	6	0	2.442103	2.250679	6.234622
59	1	0	2.597526	1.994572	7.277113
60	6	0	1.870369	3.474484	5.882233
61	1	0	1.571705	4.168352	6.663182
62	6	0	4.723970	0.179708	6.294283
63	6	0	4.915759	-0.517383	7.499294
64	1	0	4.114265	-1.128864	7.899902
65	6	0	6.131679	-0.412062	8.180835
66	1	0	6.271758	-0.950983	9.112166
67	6	0	7.155848	0.400457	7.678750
68	1	0	8.094880	0.487489	8.214567
69	6	0	1.286314	6.667096	-2.658181
70	1	0	0.837783	7.125665	-3.553589
71	1	0	2.125240	7.317500	-2.379146
72	6	0	2.674253	5.222282	-4.151182
73	1	0	3.459982	5.984040	-4.069778
74	1	0	2.113218	5.450079	-5.078664
75	6	0	3.299069	3.848190	-4.260441
76	6	0	2.702220	2.843010	-5.037405
77	1	0	1.806523	3.069999	-5.609615
78	6	0	3.254697	1.561170	-5.109488
79	1	0	2.792130	0.798159	-5.725994
80	6	0	4.423493	1.256045	-4.393074
81	6	0	5.028049	2.255709	-3.610179
82	1	0	5.932124	2.024867	-3.057549
83	6	0	4.468451	3.531899	-3.547685
84	1	0	4.935309	4.292526	-2.929496
85	7	0	-4.300532	5.562373	-0.750121
86	7	0	-7.411989	-0.040363	-0.369024
87	7	0	0.596781	5.258582	2.814669
88	7	0	3.465349	0.099292	5.595080
89	7	0	1.839818	5.327382	-2.942757
90	1	0	-5.269403	5.741349	-0.494431
91	1	0	-0.174499	4.615509	2.648169
92	1	0	1.143046	4.588920	-2.877169
93	6	0	0.957789	-6.717536	-0.063734
94	6	0	-0.000761	-6.622899	0.971744
95	6	0	-1.386417	-6.598912	0.679218
96	6	0	-1.807048	-6.715342	-0.661635
97	6	0	-0.855130	-6.782636	-1.710301
98	6	0	0.527904	-6.804643	-1.408368
99	6	0	2.449576	-6.727907	0.221071
100	1	0	2.708345	-6.457476	1.249007
101	1	0	2.949217	-6.026194	-0.454278
102	1	0	2.884893	-7.720999	0.044599

103	6	0	-2.435743	-6.461539	1.771215
104	1	0	-3.296619	-5.912345	1.379677
105	1	0	-2.076399	-5.908563	2.645666
106	1	0	-2.782211	-7.440671	2.130617
107	6	0	-1.341098	-6.828156	-3.150552
108	1	0	-0.590306	-6.462841	-3.850103
109	1	0	-2.229951	-6.207719	-3.289959
110	1	0	-1.606013	-7.848088	-3.459316
111	6	0	1.592269	-6.936547	-2.496201
112	1	0	2.323323	-7.689867	-2.183184
113	1	0	1.146213	-7.322917	-3.424107
114	6	0	1.639327	-4.656602	-3.535252
115	1	0	0.730636	-4.358076	-3.000015
116	1	0	1.314559	-5.078604	-4.506454
117	6	0	2.511534	-3.447229	-3.780210
118	6	0	2.359713	-2.271973	-3.028041
119	1	0	1.594681	-2.227338	-2.257495
120	6	0	3.174034	-1.160897	-3.246517
121	1	0	3.041171	-0.262639	-2.654720
122	6	0	4.177108	-1.193908	-4.235545
123	6	0	4.334643	-2.369757	-4.996568
124	1	0	5.089309	-2.404969	-5.773481
125	6	0	3.512580	-3.472948	-4.767206
126	1	0	3.634150	-4.358316	-5.387008
127	6	0	6.386848	-0.201419	-4.773870
128	6	0	7.170209	-1.169973	-4.118101
129	1	0	6.714468	-1.810217	-3.371176
130	6	0	8.527017	-1.301925	-4.423934
131	1	0	9.118673	-2.053289	-3.910152
132	6	0	9.128582	-0.462743	-5.369716
133	1	0	10.183892	-0.563407	-5.599567
134	6	0	8.353547	0.508742	-6.014578
135	1	0	8.805965	1.162685	-6.753267
136	6	0	6.992069	0.637096	-5.728172
137	1	0	6.394048	1.382228	-6.240067
138	6	0	0.447326	-6.578666	2.409227
139	1	0	-0.330714	-6.900659	3.099674
140	1	0	1.338067	-7.177952	2.600447
141	6	0	1.042903	-4.952951	4.370911
142	1	0	1.677447	-5.790525	4.671225
143	1	0	0.052472	-5.081050	4.817260
144	6	0	1.668722	-3.631624	4.678252
145	6	0	0.899080	-2.452710	4.750752
146	1	0	-0.179592	-2.497450	4.613642
147	6	0	1.485032	-1.225377	5.034193
148	1	0	0.870733	-0.336667	5.100817
149	6	0	2.879356	-1.127297	5.279443
150	6	0	3.653131	-2.313054	5.202968
151	1	0	4.719787	-2.267189	5.379477
152	6	0	3.055369	-3.531647	4.907697
153	1	0	3.676021	-4.423670	4.865567
154	6	0	5.749811	0.994680	5.790818
155	1	0	5.594682	1.539746	4.866491
156	6	0	6.957816	1.105731	6.485667

157	1	0	7.745143	1.739657	6.091498
158	6	0	-3.298480	-6.763745	-0.960841
159	1	0	-3.476011	-7.201759	-1.954505
160	1	0	-3.790538	-7.441242	-0.250601
161	6	0	-5.353953	-5.369418	-1.190610
162	1	0	-5.895403	-6.091205	-0.567200
163	1	0	-5.507735	-5.681514	-2.241384
164	6	0	-5.912407	-3.981184	-0.978758
165	6	0	-5.710619	-2.972570	-1.936124
166	1	0	-5.190979	-3.206265	-2.862553
167	6	0	-6.196079	-1.679188	-1.739807
168	1	0	-6.046794	-0.919417	-2.498426
169	6	0	-6.906675	-1.356027	-0.567474
170	6	0	-7.110635	-2.361556	0.397706
171	1	0	-7.655480	-2.127039	1.304961
172	6	0	-6.618910	-3.650036	0.188958
173	1	0	-6.782635	-4.410505	0.947358
174	7	0	2.333989	-5.677216	-2.717327
175	7	0	4.997801	-0.056904	-4.465544
176	7	0	-3.925567	-5.436833	-0.807010
177	1	0	3.277550	-5.842022	-3.061888
178	1	0	-3.381035	-4.691140	-1.237226
179	1	0	0.076606	-4.500435	2.530974
180	1	0	1.671406	-4.850110	2.348084
181	7	0	0.817842	-5.139640	2.841362

Picrate

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.816351	1.217248	0.007162
2	6	0	-1.512722	-0.000886	0.019833
3	6	0	-0.814897	-1.218186	0.007250
4	6	0	0.562784	-1.224927	-0.018820
5	6	0	1.386109	0.000879	-0.096353
6	6	0	0.561327	1.225575	-0.018853
7	1	0	-1.360181	2.151713	0.025194
8	1	0	-1.357616	-2.153292	0.025441
9	8	0	2.627394	0.001589	-0.281195
10	7	0	1.193864	2.528030	0.006472
11	7	0	1.196916	-2.526614	0.006493
12	7	0	-2.940344	-0.001748	0.070678
13	8	0	2.372908	2.639372	0.448062
14	8	0	0.512456	3.532810	-0.401501
15	8	0	0.516752	-3.532242	-0.401504
16	8	0	2.376087	-2.636585	0.448126
17	8	0	-3.555507	1.118146	0.091840
18	8	0	-3.554183	-1.122381	0.091490

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