

## Supporting Information

# **Femtosecond to Nanosecond Dynamics of 2,2'-Bipyridine-3,3'-diol inside the Nano-Cavities of Molecular Containers**

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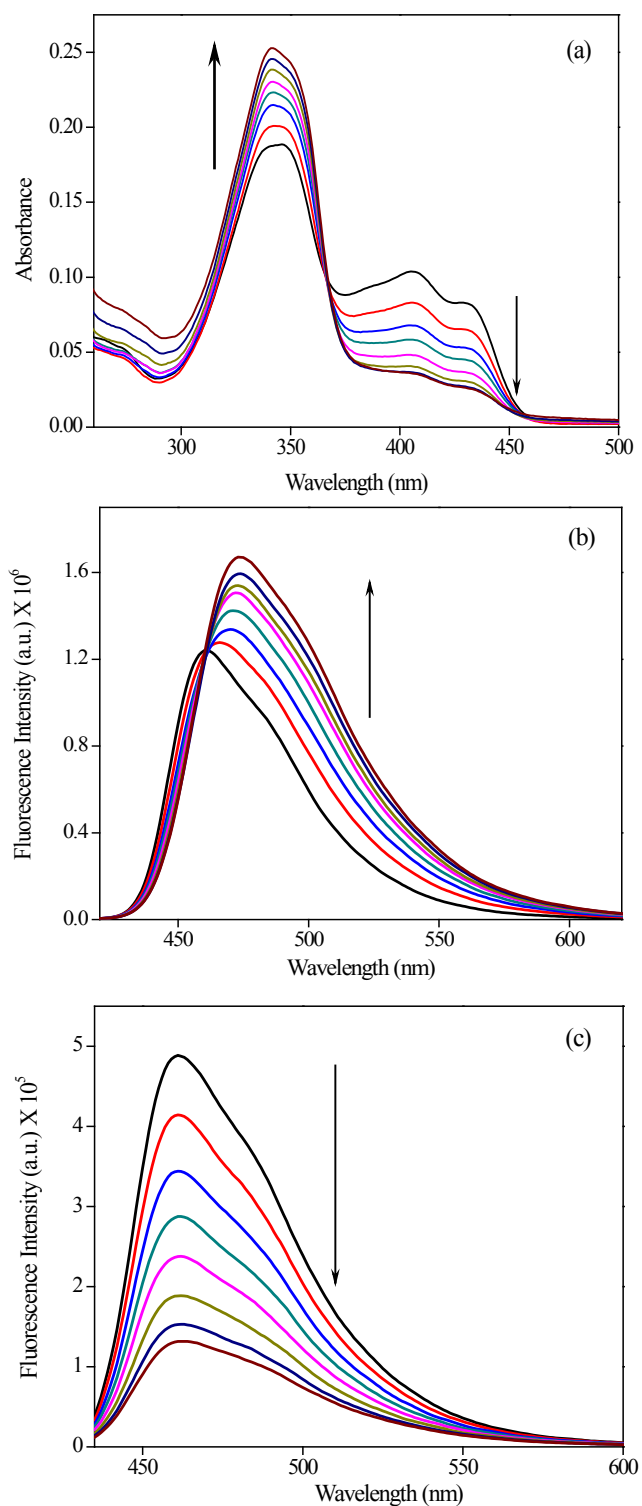
**Table S1.** Fluorescence decay transients (measured in TCSPC set-up) of BP(OH)<sub>2</sub> in absence and presence of cucurbit[7]uril (CB7) collected at 465 nm ( $\lambda_{\text{ex}}=375$  nm).

[CB7]	$\tau_1$ (ns)	$a_1$	$\tau_2$ (ns)	$a_2$	$\tau_{\text{avg}}^{\#}$	$\chi^2$
0	0.63	1	-	-	0.63	1.09
30 $\mu\text{M}$	0.64	0.92	8.43	0.08	1.26	1.01
60 $\mu\text{M}$	0.67	0.84	8.56	0.16	1.93	1.08
100 $\mu\text{M}$	0.68	0.7	8.65	0.3	3.07	1.00
150 $\mu\text{M}$	0.68	0.63	8.65	0.37	3.63	0.99
200 $\mu\text{M}$	0.69	0.44	8.73	0.55	5.15	1
300 $\mu\text{M}$	0.69	0.32	8.71	0.68	6.16	1.03
400 $\mu\text{M}$	0.69	0.25	8.74	0.75	6.69	1.03
500 $\mu\text{M}$	0.69	0.17	8.73	0.83	7.37	1.04

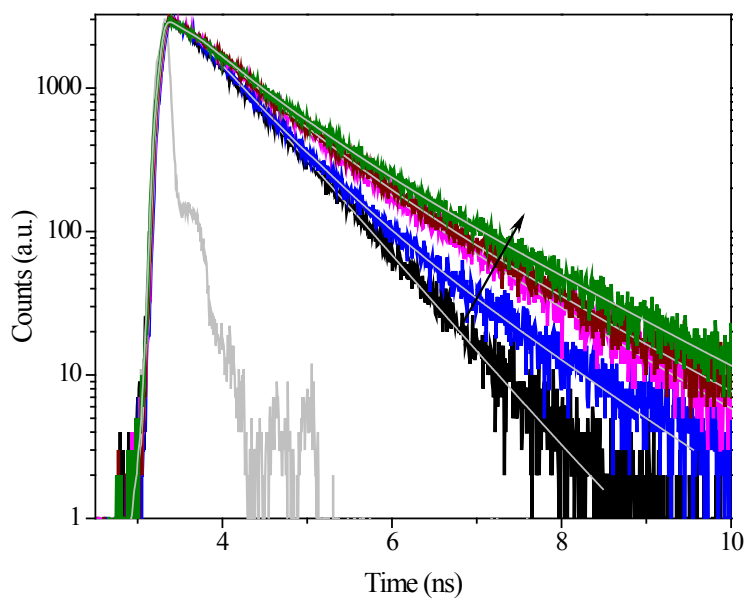
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<sup>#</sup>  $\tau_{\text{avg}} = (a_1\tau_1 + a_2\tau_2)$

**Note S1.** BP(OH)<sub>2</sub> exhibits red shift in absorption spectra in presence of CB7, however, similar red shift is absent in case of β-cyclodextrin (β-CD), indicating CB7 forms more stable inclusion complex with BP(OH)<sub>2</sub> than that of β-CD. Observations from steady-state emission studies show that the enhancement in fluorescence of BP(OH)<sub>2</sub> in CB7 is much higher than that observed in case of β-CD. Though the stoichiometry is same for both the host molecules, binding affinity is 3 times more for CB7:BP(OH)<sub>2</sub> (3000 M<sup>-1</sup>) compared to β-CD:BP(OH)<sub>2</sub> (900 M<sup>-1</sup>). Pico-second time resolved study indicates that BP(OH)<sub>2</sub> exhibits bi-exponential fluorescence decay in both the hosts. But the lifetime of BP(OH)<sub>2</sub> in CB7 complex (~8.5 ns) is much higher than that of β-CD (~5 ns). This further confirms that stability of BP(OH)<sub>2</sub> in BP(OH)<sub>2</sub>:CB7 complex is higher than that in BP(OH)<sub>2</sub>:β-CD. Therefore, all the above results conclude that the behaviour of nano-cavity is different for CB7 from β-CD.



**Figure S1.** Absorption (a) and Emission (b) ( $\lambda_{\text{ex}}=345$  nm), (c) ( $\lambda_{\text{ex}}=425$  nm) spectra of BP(OH)<sub>2</sub> in presence of 0 to 14 mM of  $\beta$ -CD. Arrow indicates the direction of increase in  $\beta$ -CD concentration.



**Figure S2.** Fluorescence decay overlays of  $\text{BP(OH)}_2$  in presence of  $\beta$ -CD (from 0 to 14 mM) collected at 465 nm ( $\lambda_{\text{ex}}=375$  nm). Arrow indicates the direction of increase in  $\beta$ -CD concentration.