Supporting Information

A Novel Photo-Responsive Azobenzene-Containing Nano-Ring Host for Fullerene Guest Facile Encapsulating and Releasing

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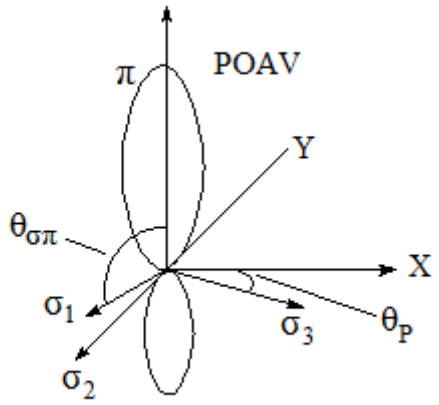


Figure S1. π-orbital axis vector (POAV) shown for a nonplanar conjugated carbon atom bonded to atoms 1, 2, 3, through the schematized σ bonds σ_1, σ_2, σ_3, and definition of the angles $\theta_{\sigma\pi}$ made by the π-orbital to each of the σ bonds.

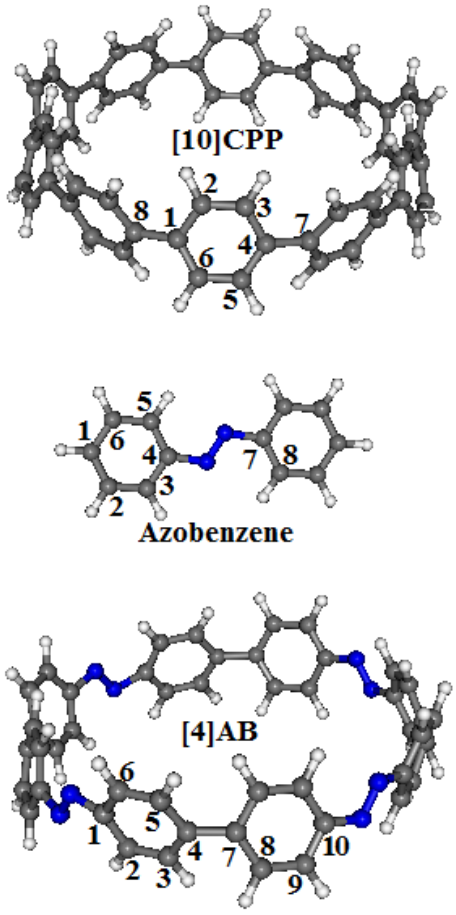


Figure S2. Atom label of the [10]CPP, azobenzene and [4]AB for POVA listed in Table S1

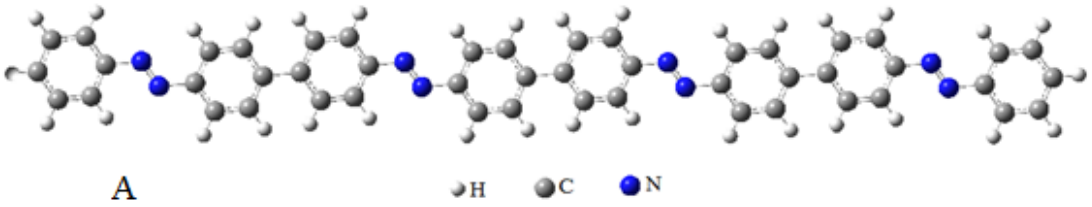
Table S1 the θ_p (°) of some selected C atom (see Figure S2) of the azobenzene, [10]CPP and [4]AB nanoring

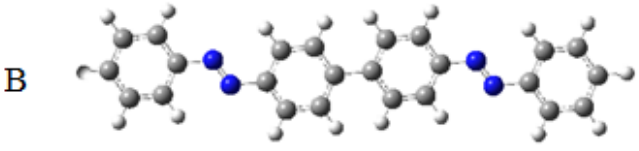
Atom lable	1	2	3	4	5	6	7	8	9	10
[10]CPP	3.89	2.45	2.45	3.88	1.09	1.11	3.87	3.91	–	–
Azobenzene	0	0	0	0	0	0	0	0	–	–
[4]AB	4.10	2.29	2.30	3.82	1.42	1.55	3.84	1.43	1.58	4.00

Equation S1

$Strain=E_0-E_A-(E_B-2E_C)$ Eq(S1)

Where E_0 is the energy of the free [4]AB nanoring, E_A is the energy of the open-ring structure (**A**) of the [4]AB, E_B is the energy of the open-ring structure (**B**) of the [2]AB, E_C is the energy of the azobenzene (**C**). For clarity, the structures of **A**, **B** and **C** are given below.





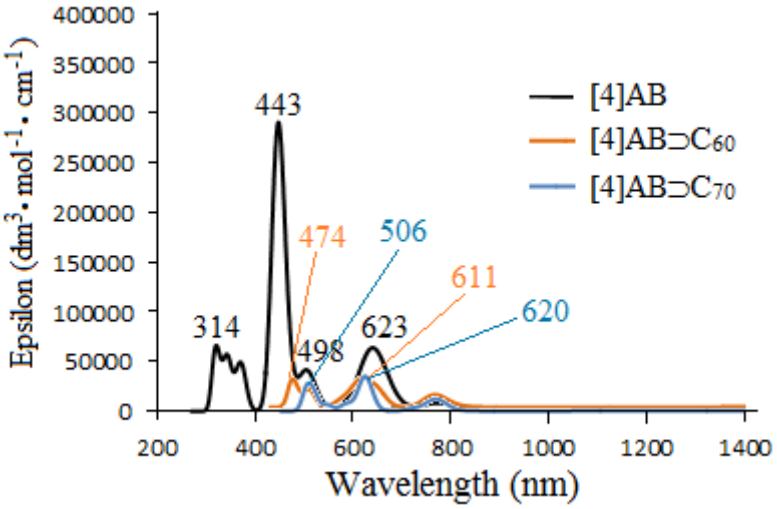


Figure S3. Simulated UV-visible-NIR absorption spectrum compare for the *trans*-[4]AB, [4]AB⊃C_{60} and [4]AB⊃C_{70} host-guest complexes