Electronic Supplementary Information (ESI)

Electron transfer photochromism of solid-state supramolecules constructed by cucurbit[n]uril (n = 5-8) and 1-(4-carboxybenzyl)-4-[2-(4-pyridyl)-vinyl]-pyridinium chloride

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Figure S1. 2D gCOSY NMR spectrum of $\mathbf{1}^{+}$ with 1.10 equiv. of Q[5] at pD 2.0.

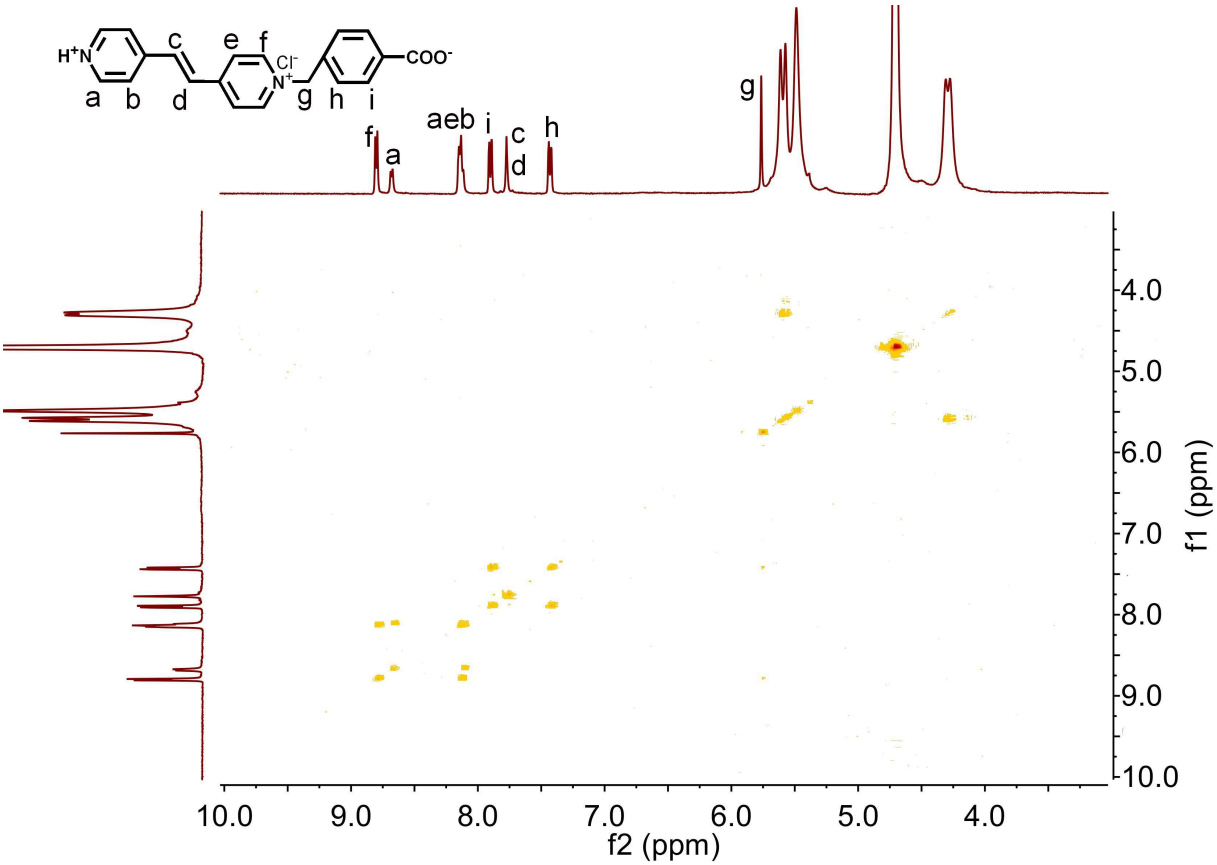

Figure S2. 2D gCOSY NMR spectrum of $\mathbf{1}^{+}$ with 1.10 equiv. of Q[6] at pD 2.0.

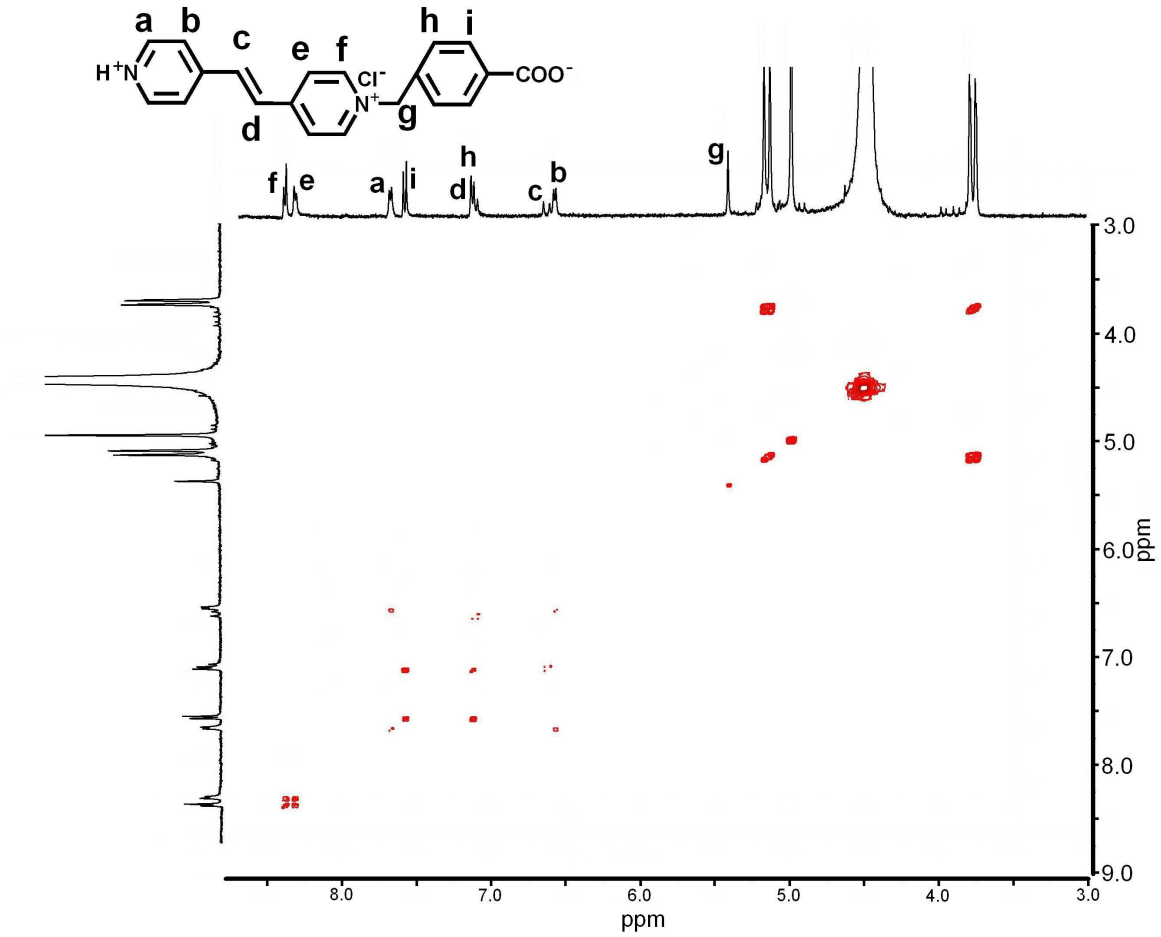

Figure S3. 2D gCOSY NMR spectrum of $\mathbf{1}^{+}$ with 1.12 equiv. of Q[8] at pD 2.0.

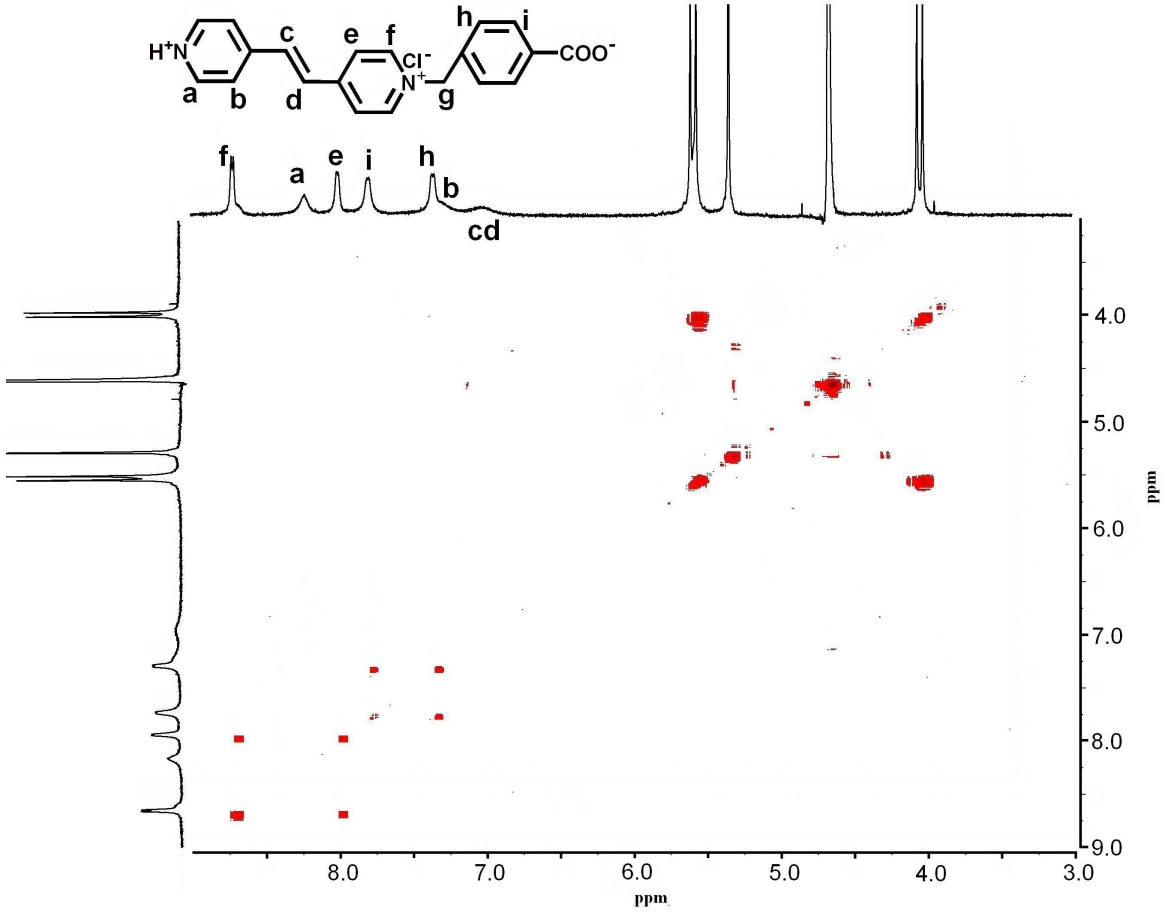

Figure S4. ^{1}H NMR spectra of 1^{+} (A) with 1.12 equiv of Q[8] before (B) and after (C) irradiation.

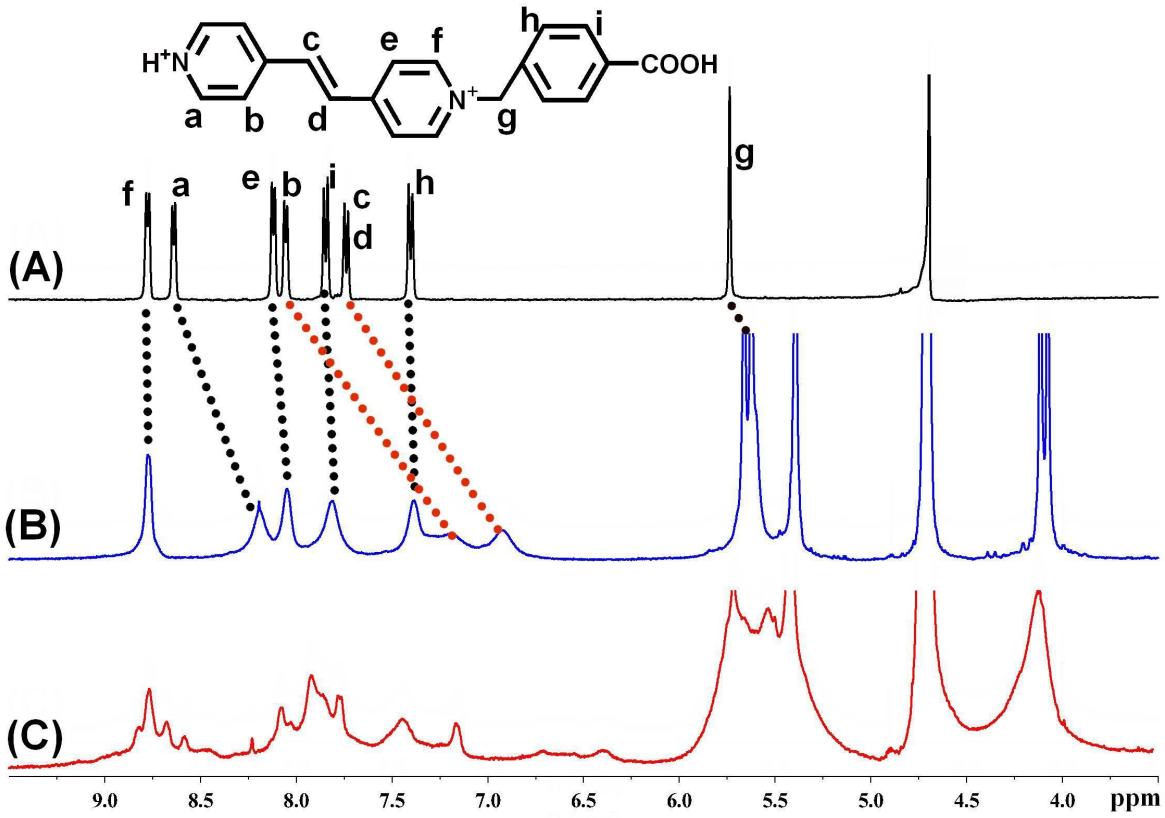

Figure S5. UV-Vis spectra of 1^{+}_{2}@Q[8] before and after irradiation.

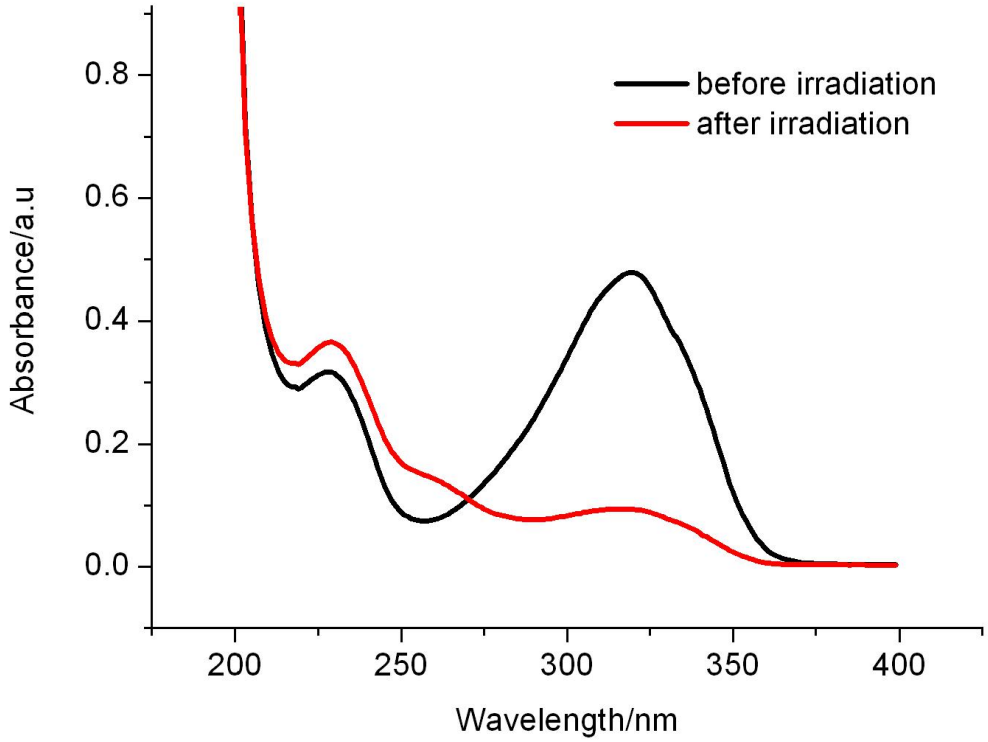

Figure S6. Left column, change in absorption spectra of guest **1** with increasing concentration of Q[*n*]. Right column, the curves of Absorbance *vs.* $N_{Q[n]}/N_{guest}$.

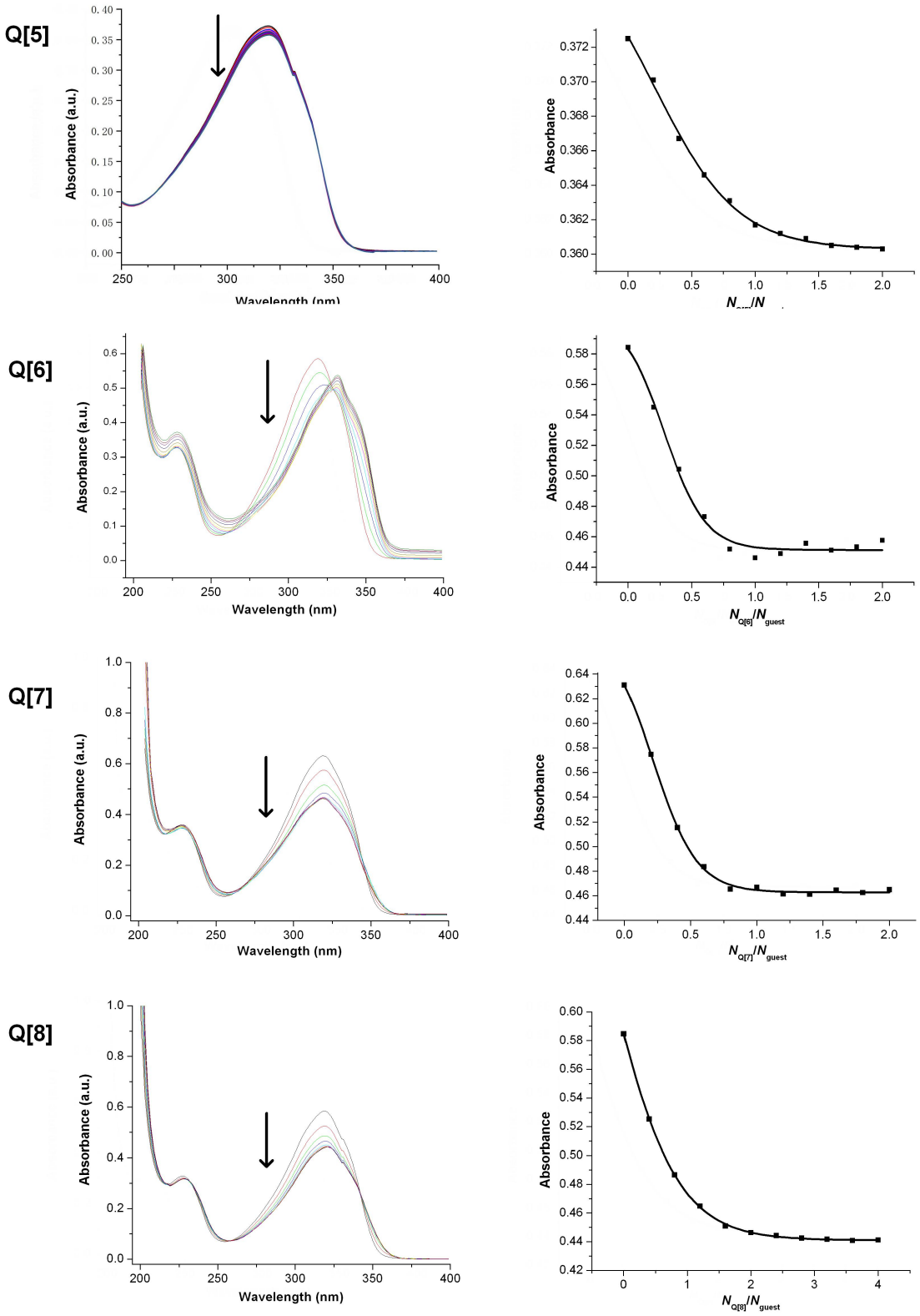

Table S1. Binding ratios and binding constants of $\mathbf{1}^{+}\cdot Cl^{-}$ with Q[*n*]s.

Host	Q[5]	Q[6]	Q[7]	Q[8]
Binding ratios	1:1	1:1	1:1	1:2
Binding constants (*K*a, M^{-1})	$(3.65\pm0.80)*10^{3}$	$(1.80\pm0.60)*10^{4}$	$(2.91\pm0.72)*10^{4}$	$(4.50\pm0.09)*10^{4}$

Figure S7. Photos showing the colour change can occur multiple times.

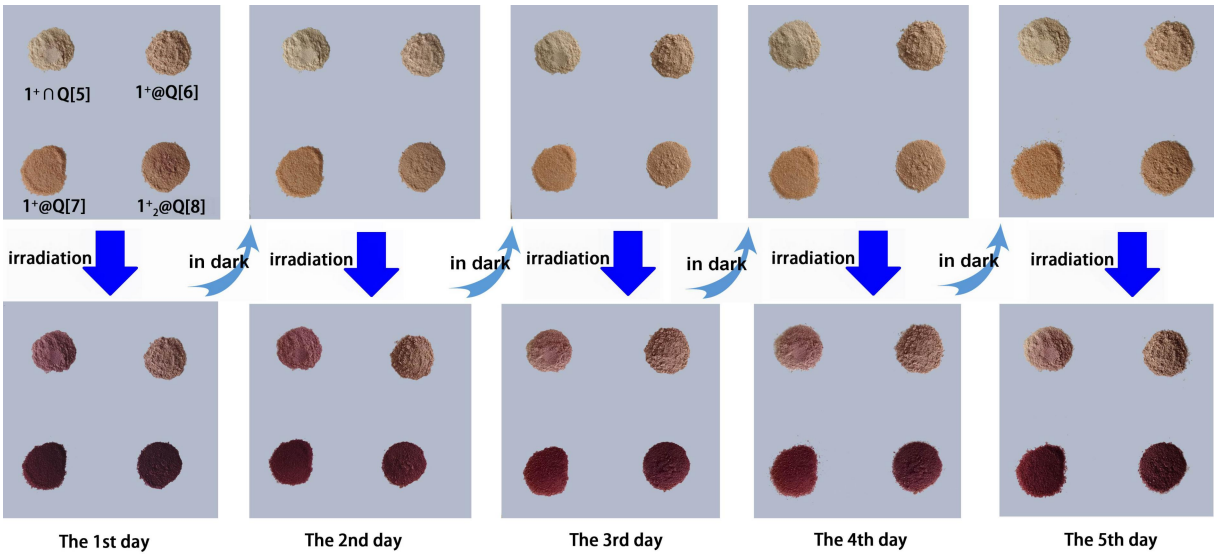

Figure S8. IR spectra of $\mathbf{1}^{+}$@Q[7] before and after irradiation.

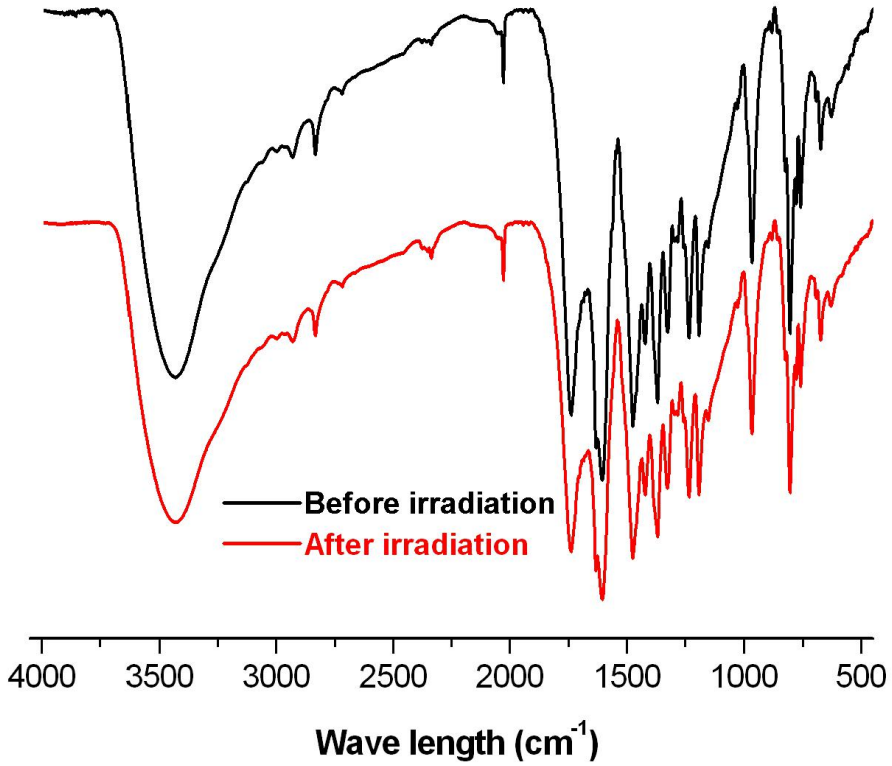

Figure S9. IR spectra of inclusion complex $\mathbf{1}^{+}_{2}$@Q[8] before and after irradiation.

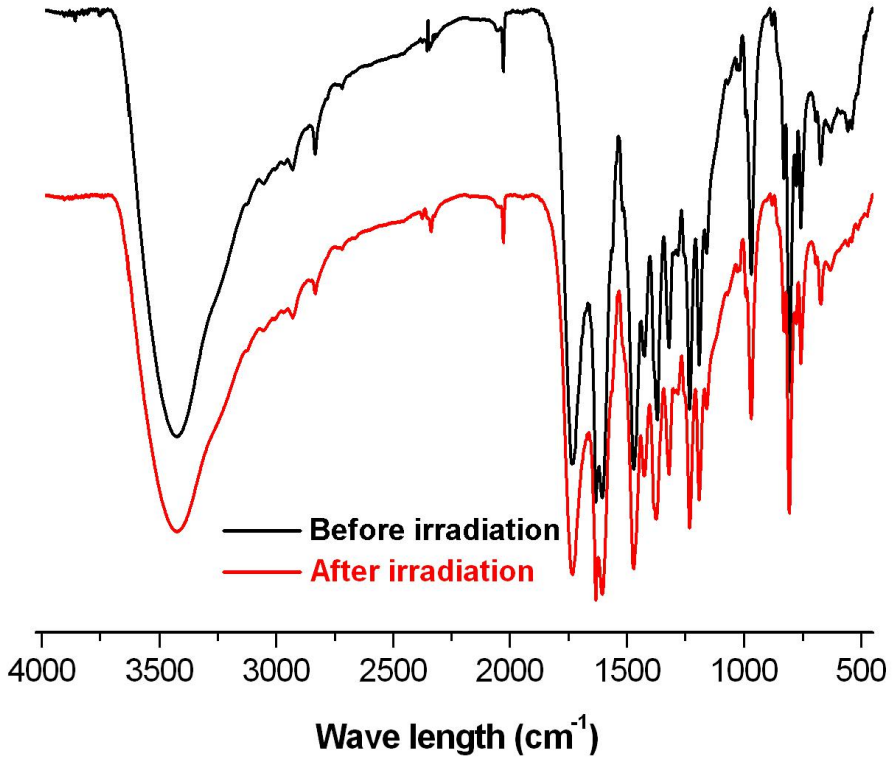

Figure 10. Energy minimized structures of four complexes $\mathbf{1}^{+}\cap$Q[5], $\mathbf{1}^{+}$@Q[6], $\mathbf{1}^{+}$@Q[7], and $\mathbf{1}^{+}_{2}$@Q[8] in the gas phase by a HF/3-21G** calculation.