Electronic Supplementary Information (ESI)

Light-responsive molecular switch based on cucurbit[7]uril and 1,1'-bis(benzyl)-4-[2-(4-pyridyl)-vinyl]-pyridinium dibromide displaying white light emission

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X-ray Crystallography

Crystal structure Determination: Single crystal X-ray data of $\mathbf{1}^{2+}\cdot[ZnCl_4]^{2-}\cdot H_2O$ were collected on a Bruker Apex-2000 diffractometer at 296 K using graphite monochromated Mo-*K*α radiation (λ = 0.71073 Å) with ω/2θ scan mode. Lorentz-polarization and absorption corrections were applied. Structural solution and full matrix least-squares refinement based on F^2 were performed with the SHELXS-97 and SHELXL-97 program package[1-3], respectively. All the non-hydrogen atoms were refined anisotropically. The idealized positions of the hydrogen atoms were located by using 'riding' model with $U_{iso} = 1.2U_{eq}$ of carrier atom. Analytical expressions of neutral-atom scattering factors were employed, and anomalous dispersion corrections were incorporated.

Crystal data for guest 1 ($\mathbf{1}^{2+}\cdot[ZnCl_4]^{2-}\cdot H_2O$): Empirical formula $C_{52}H_{52}Zn_2Cl_8N_4O_2$, *Mr* = 1179.32, Monoclinic, space group $P2_1/n$, *a* = 10.3073(18) Å, *b* = 18.584(3) Å, *c* = 14.516(2) Å, *b* = 105.319(4) °, *V* = 2681.7(8) Å^3, *Z* = 2, *Dc* = 1.460 g·cm^{-3}, *F*(000) = 1208, *GoF* = 1.005, R_1 = 0.0457 (I>2σ(I)), wR_2 = 0.1079 (all data). Crystal structures of guest **1** are shown in Figure S8. CCDC 2054567 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Preparation of the single crystal of $\mathbf{1}^{2+}\cdot[ZnCl_4]^{2-}\cdot H_2O$: **1**[·$Br_2$] (10.5 mg, 0.02 mmol) was dissolved in a solution of 1.0 mol·L^{-1} hydrochloric acid (5.0 ml), and to this solution $ZnCl_2$ (4 mg, 0.03 mmol) and was added. The mixture was heated to dissolve and then filtered. Slow evaporation of the filtrate over a period of a month obtained colorless crystals and collected with a yield of 70%.

References

1. Sheldrick, G. M. SHELXS-97, Program for X-ray Crystal Structure Determination, University of Göttingen, Germany, 1997.

2 Sheldrick, G. M. SHELXL-97, Program for X-ray Crystal Structure Refinement, University of Göttingen, Germany, 1997.

3 Sheldrick, G. M. A short history of SHELX, *Acta Crystallogr., Sect. A* **2008**, *64*, 112−122.

Figure S1. ^{1}H NMR spectrum of axle molecule $\mathbf{1}^{2+}$ in D_2O.

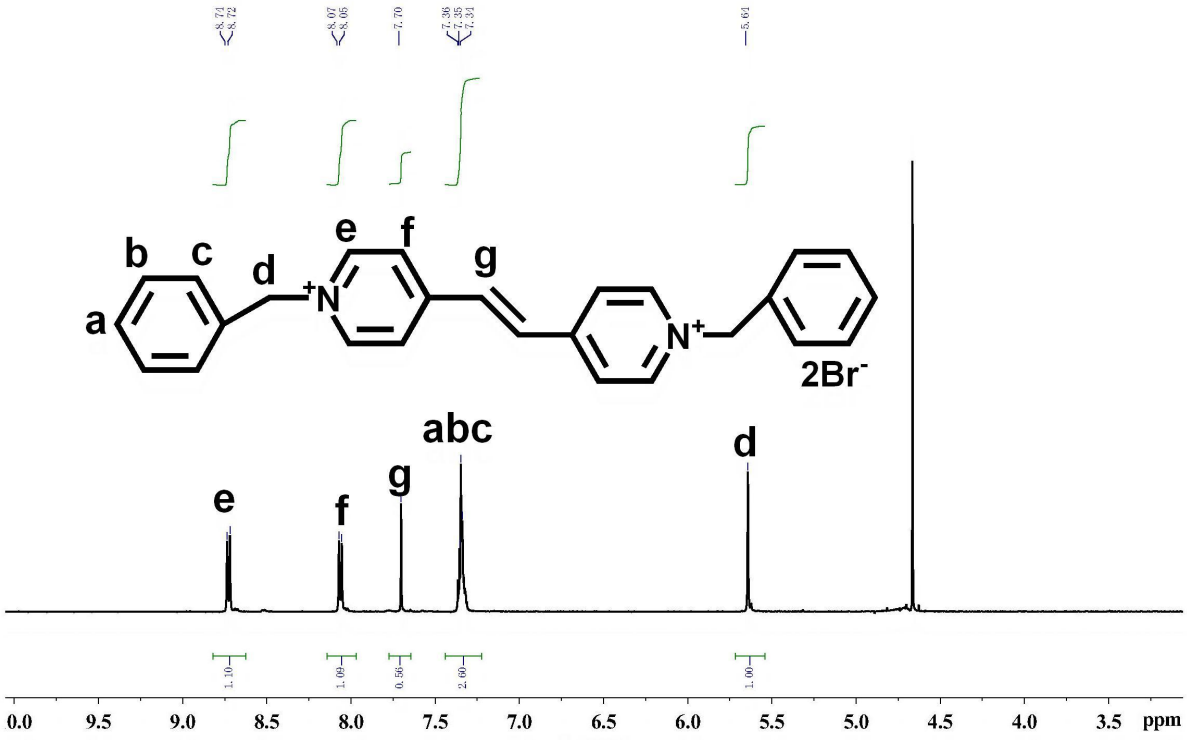

Figure S2. ^{13}C NMR spectrum of axle molecule $\mathbf{1}^{2+}$ in D_2O.

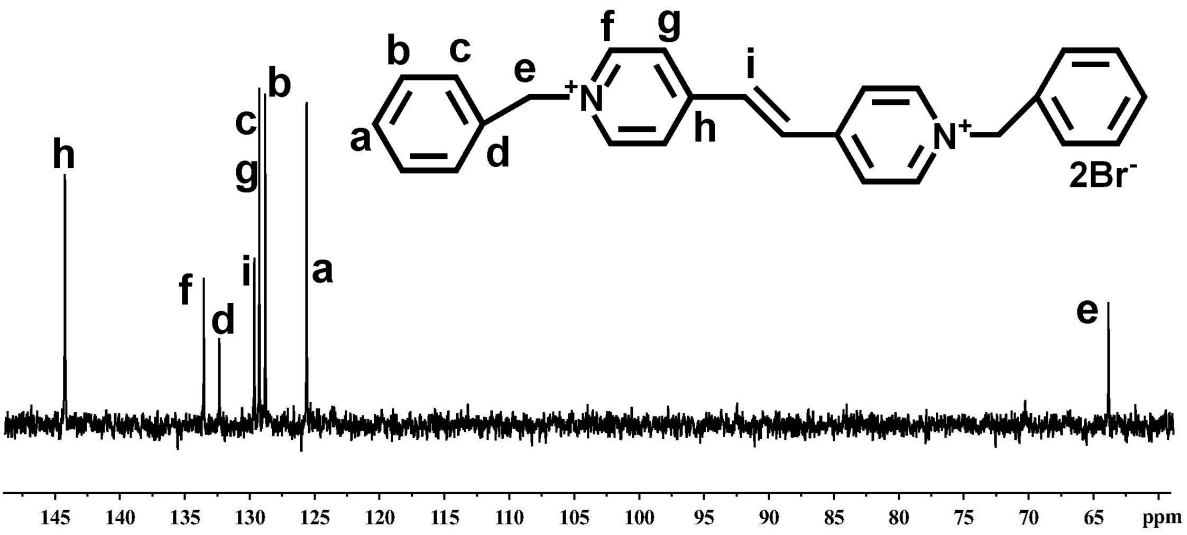

Figure S3. The high resolution mass spectrum of axle molecule $\mathbf{1}^{2+}$.

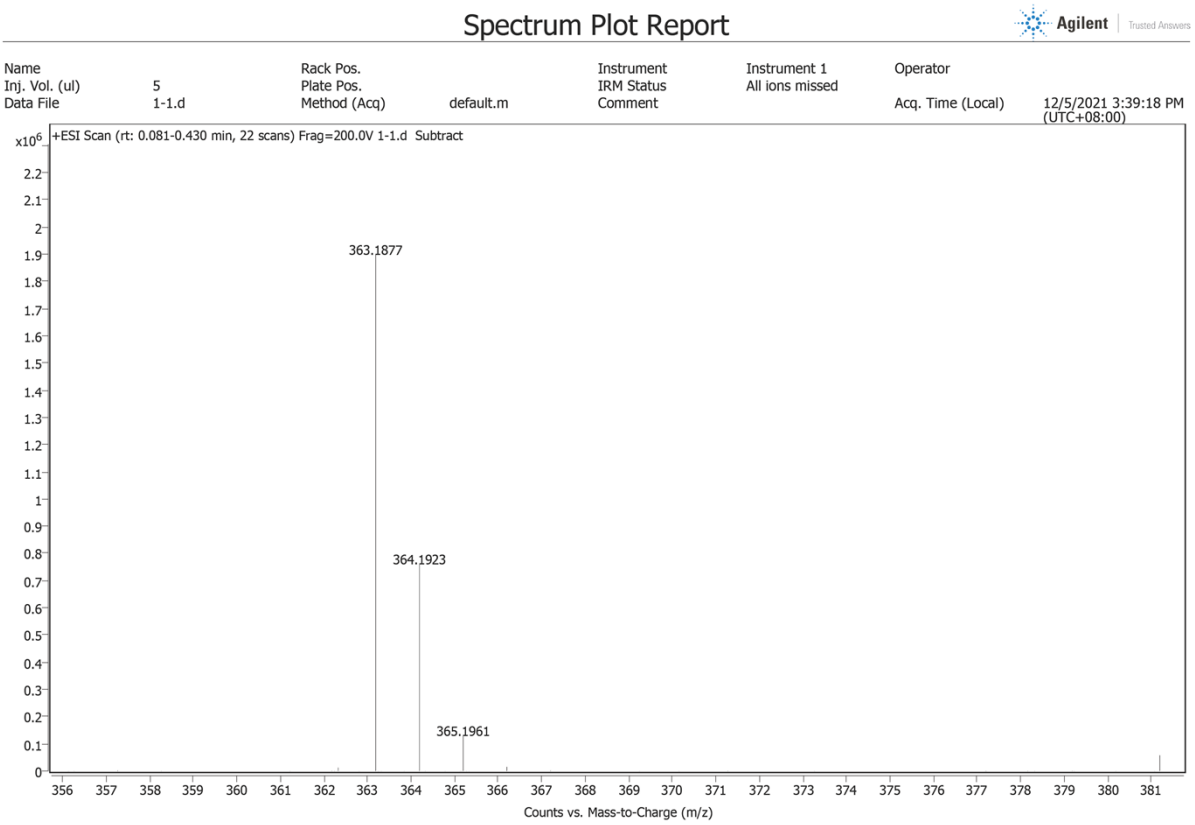

Figure S4. The ESI mass spectrum for 1:2 complex *E*-1^{2+}@Q[7]$_2$.

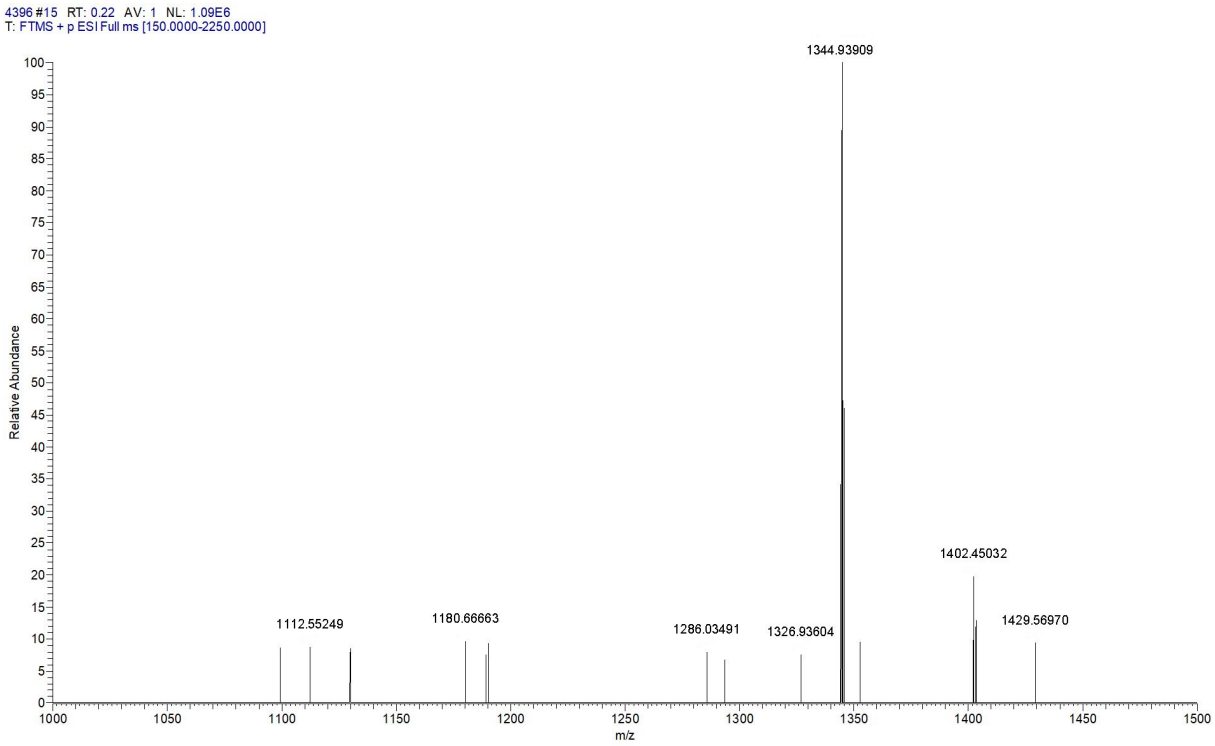

Figure S5. The ESI mass spectrum for 1:1 complex *Z*-**1**$^{2+}$@Q[7].

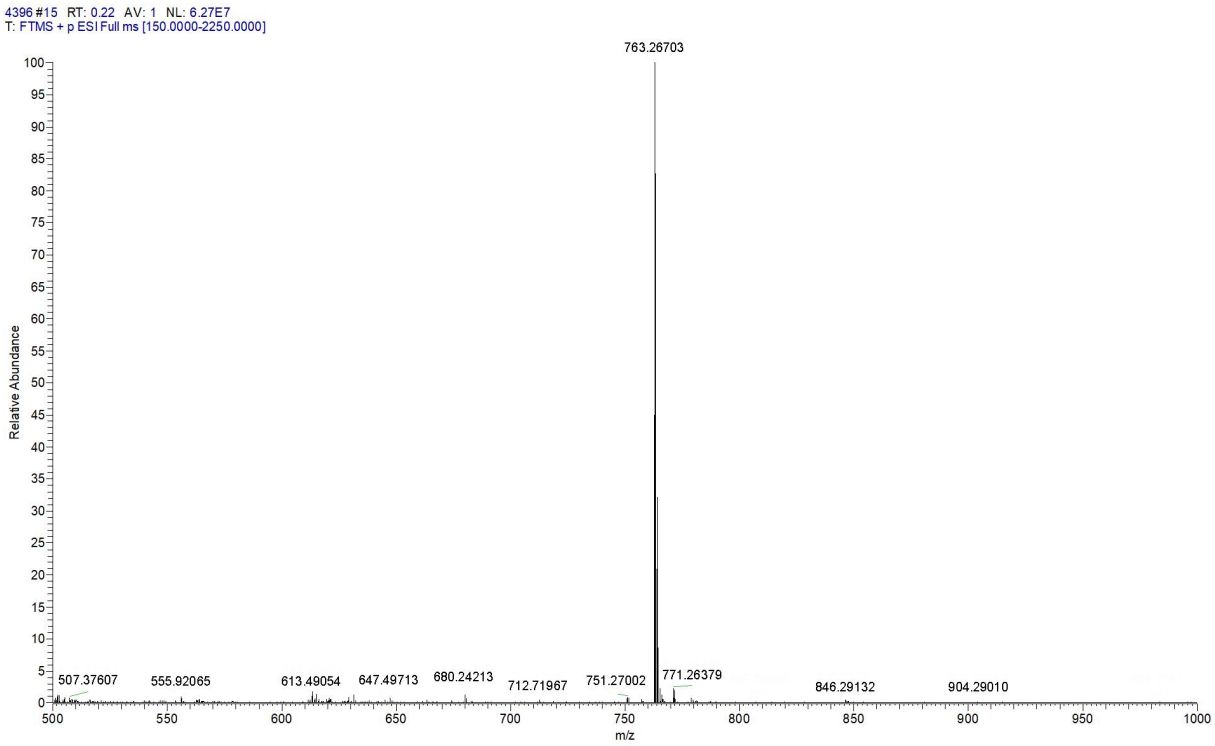

Figure S6. 2D NOESY NMR spectra of *Z*-1^{2+}@Q[7].

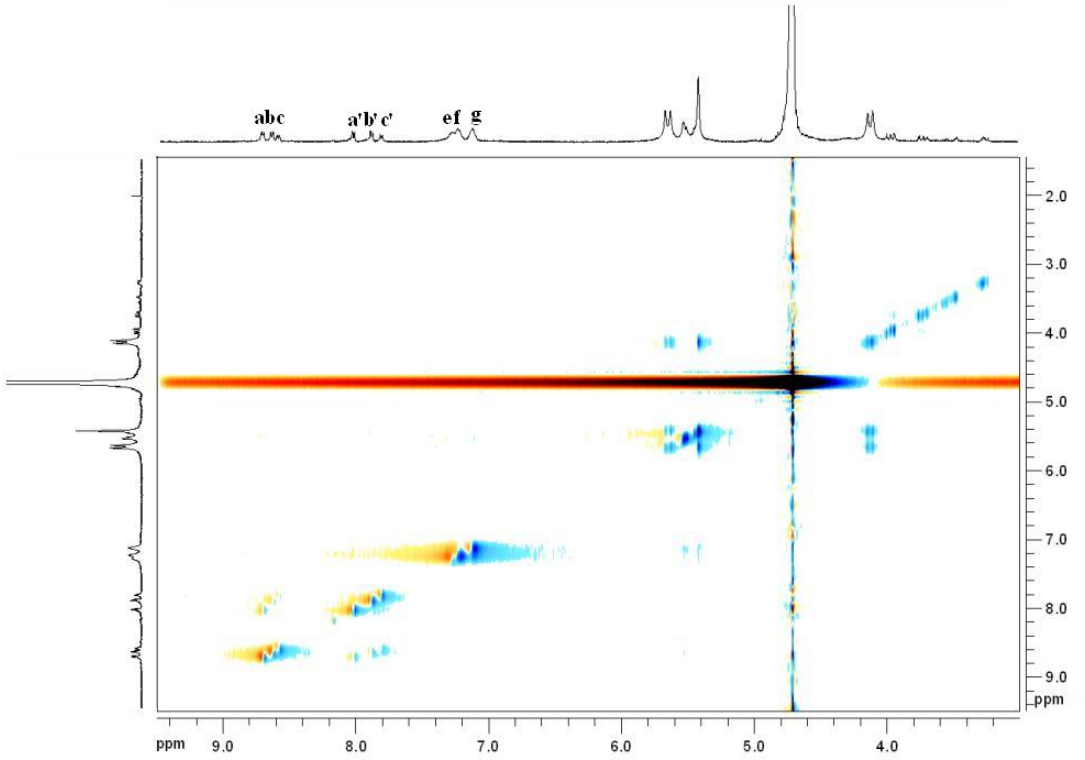

Figure S7. Fluorescence spectra of 1[·Br_2] (5.0×10^{-4} M, l_{ex} = 325 nm, left) and its inclusions $\mathbf{1}^{2+}$@Q[7]$_2$ (1.0×10^{-4} M, l_{ex} = 325 nm, right) before and after irradiation.

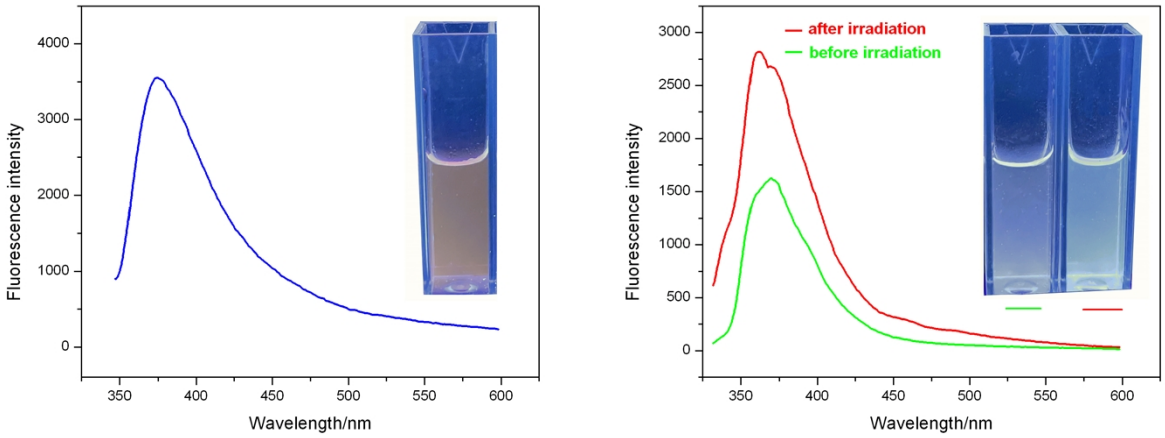

Figure S8. Crystal structure of guest **1** (**1**$^{2+}$·[$ZnCl_4$]$^{2-}$·H_2O) showing π···π interaction and C-H···π interaction between the the pyridinium and the phenyl rings of the **1**$^{2+}$.