Electronic Supplementary Material (ESI) for CrystEngComm.

Encapsulating organic guest cations in anionic MOFs that exhibit multi-responsive photochromism and photocontrolled luminescence

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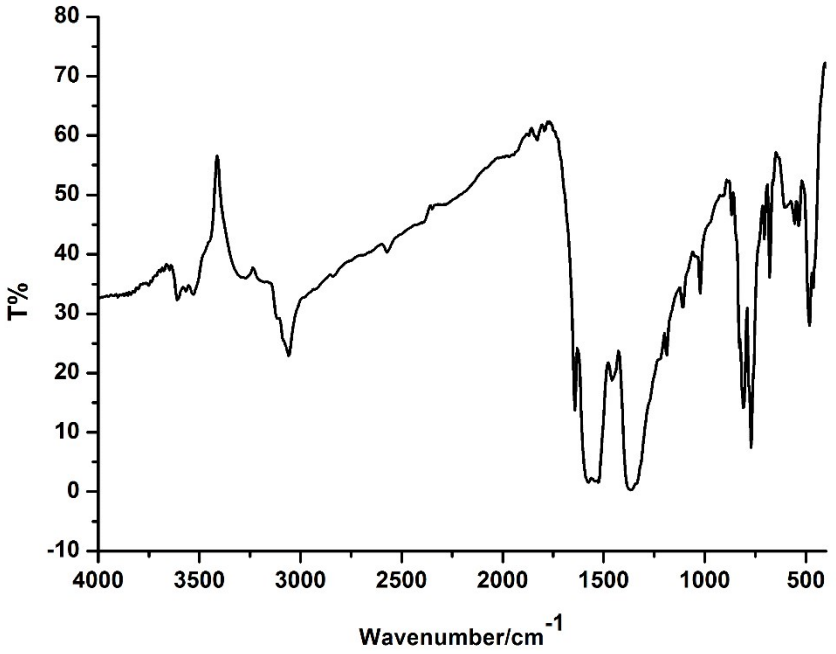

Fig. S1. IR spectrum of compound **1**.

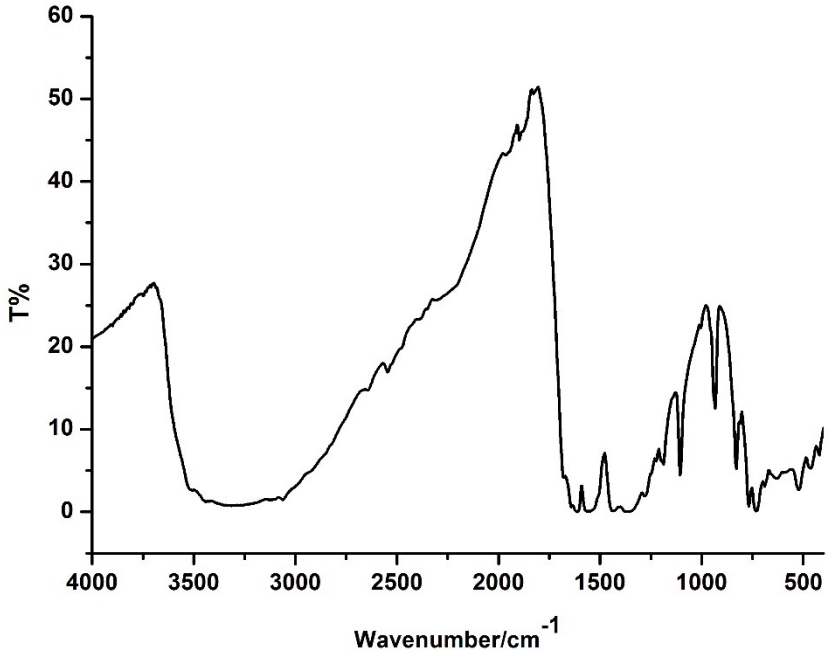

Fig. S2. IR spectrum of compound **2**.

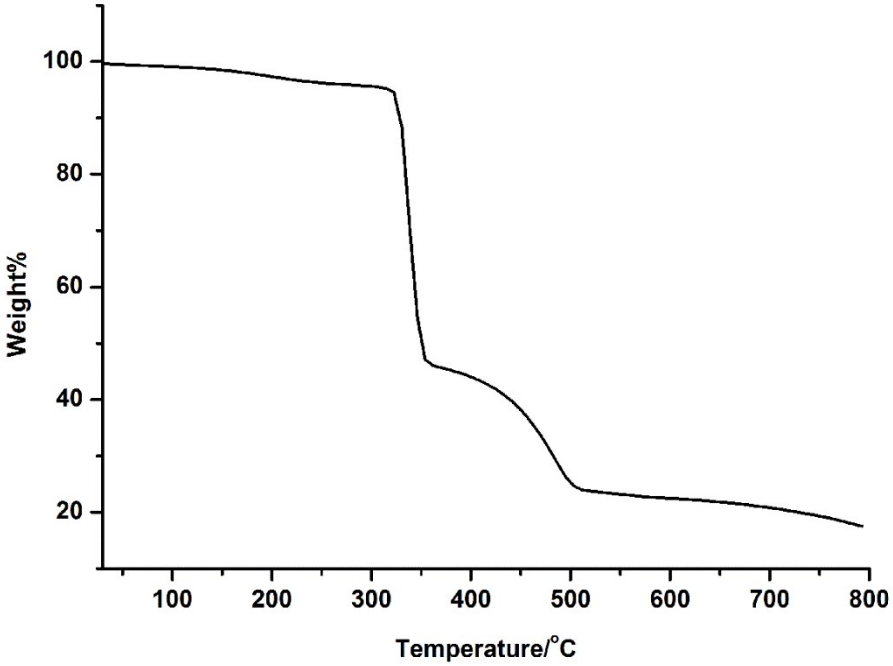

Fig. S3. TGA curve of compound **1**.

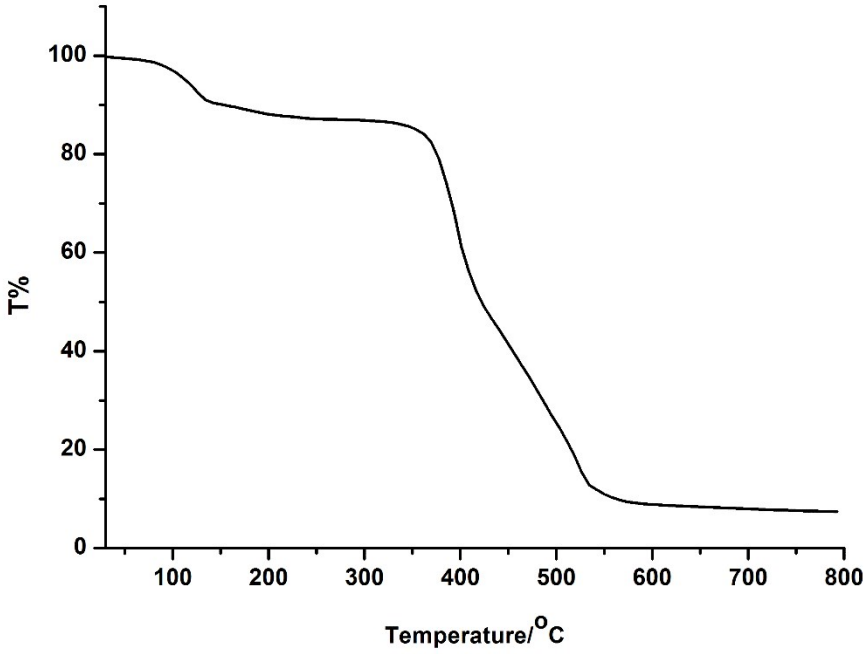

Fig. S4. TGA curve of compound **2**.

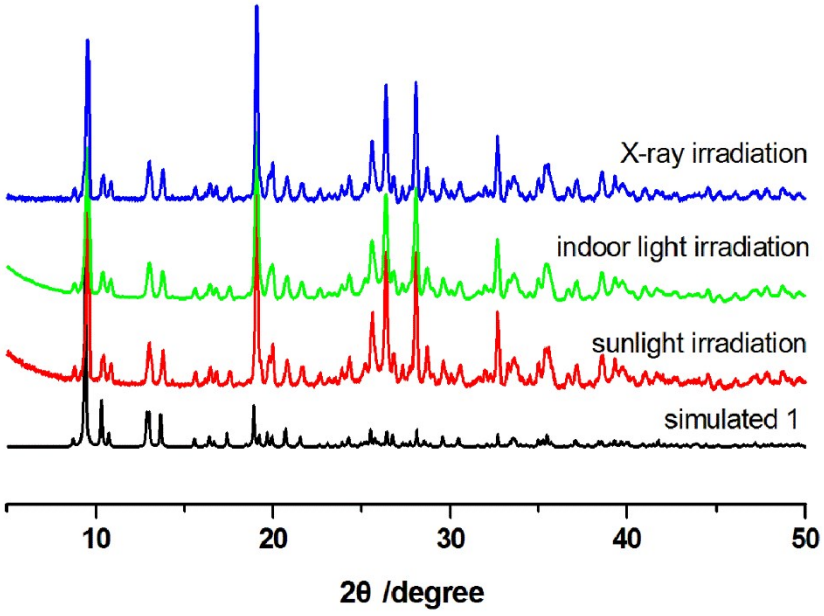

Fig. S5. PXRD patterns of compound **1** before and after irradiation.

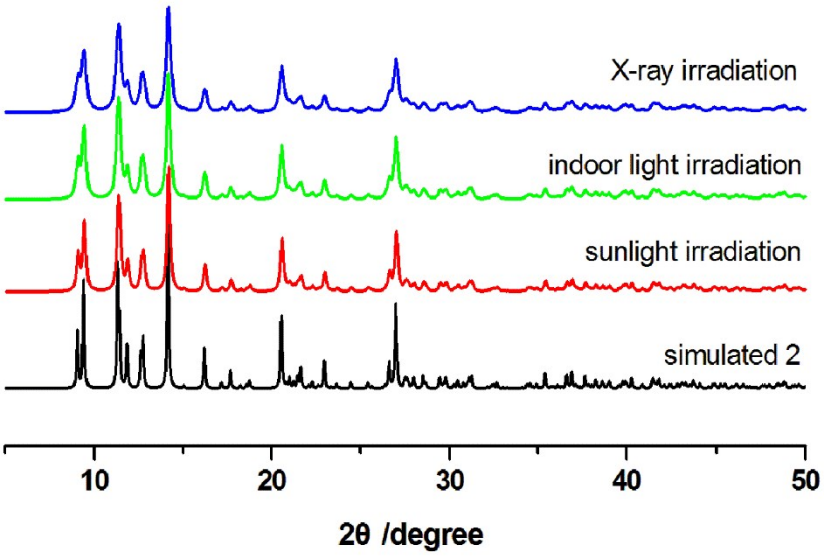

Fig. S6. PXRD patterns of compound **2** before and after irradiation.

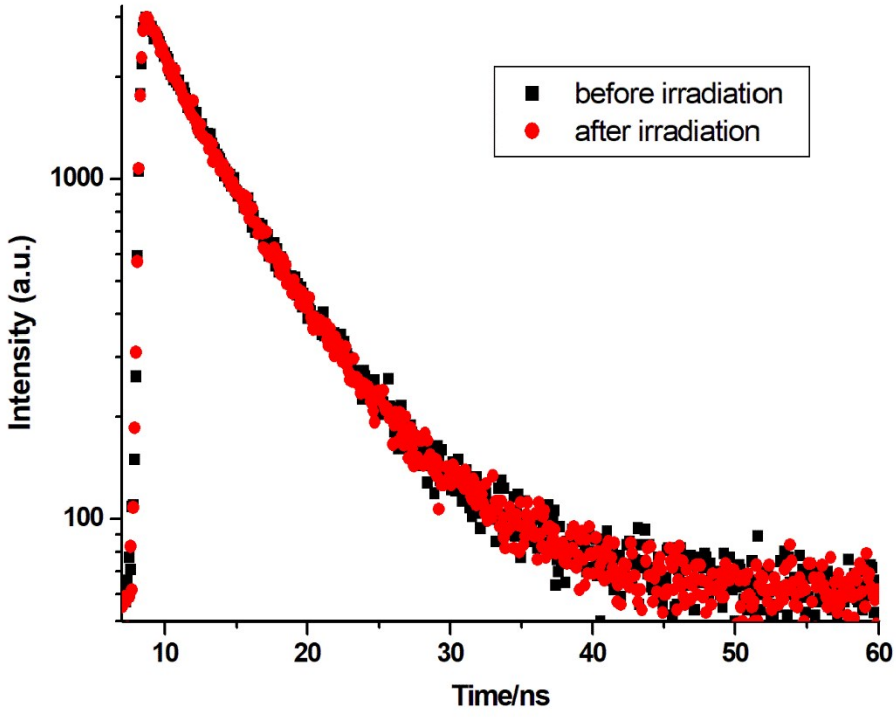

Fig. S7. Fuorescence lifetime decay curves of compound 1 before and after irradiation.

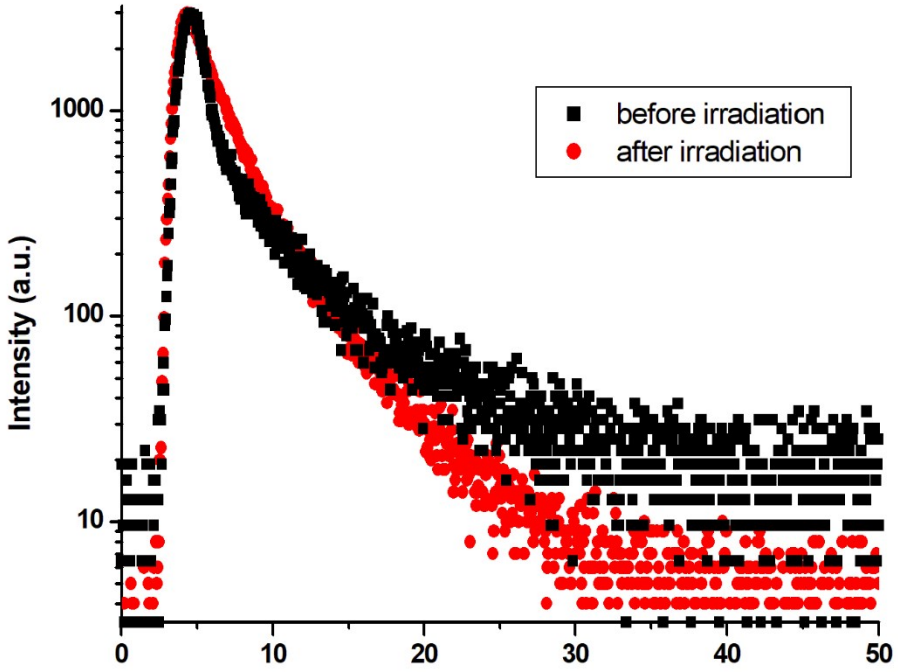

Fig. S8. Fluorescence lifetime decay curves of compound 2 before and after irradiation.

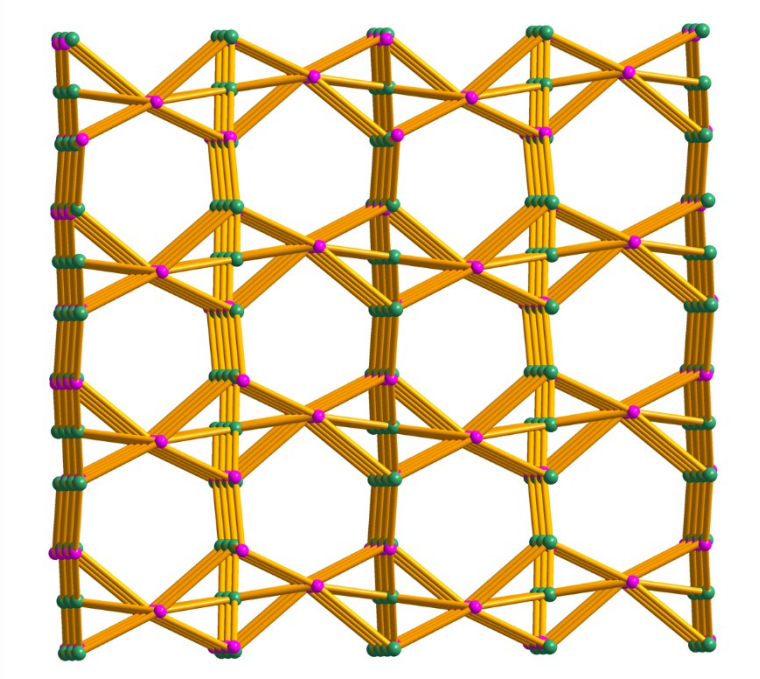

Fig. S9. Schematic representations of the (3,6)-connected framework in 1.

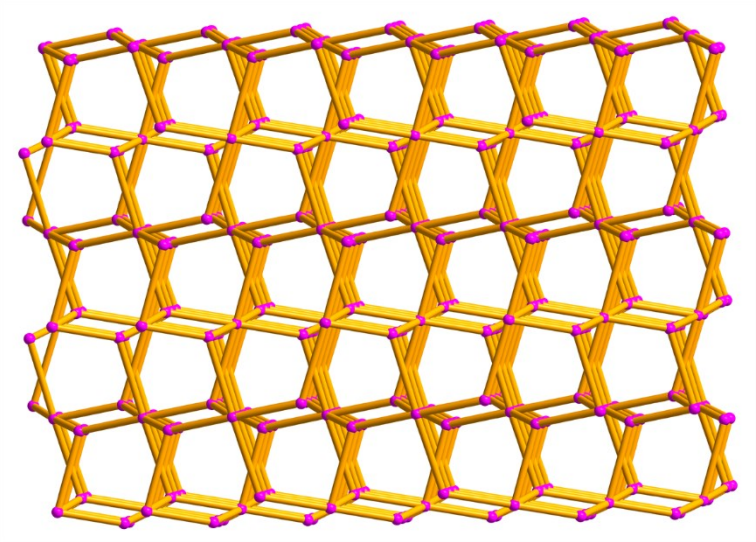

Fig. S10. Schematic representations of the (4,5,6)-connected framework in 2.

Calculation Method

First-principle calculations were performed by the density functional theory (DFT) using the Vienna Ab-initio Simulation Package (VASP) package [1]. The generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) functional were used to describe the electronic exchange and correlation effects [2-4]. Uniform G-centered k-points meshes with a resolution of $2\pi*0.04$ $Å^{-1}$ and Methfessel-Paxton electronic smearing were adopted for the integration in the Brillouin zone for geometric optimization. The simulation was run with a cutoff energy of 500 eV throughout the computations. These settings ensure convergence of the total energies to within 1 meV per atom. Structure relaxation proceeded until all forces on atoms were less than 1 meV $Å^{-1}$ and the total stress tensor was within 0.01 GPa of the target value.

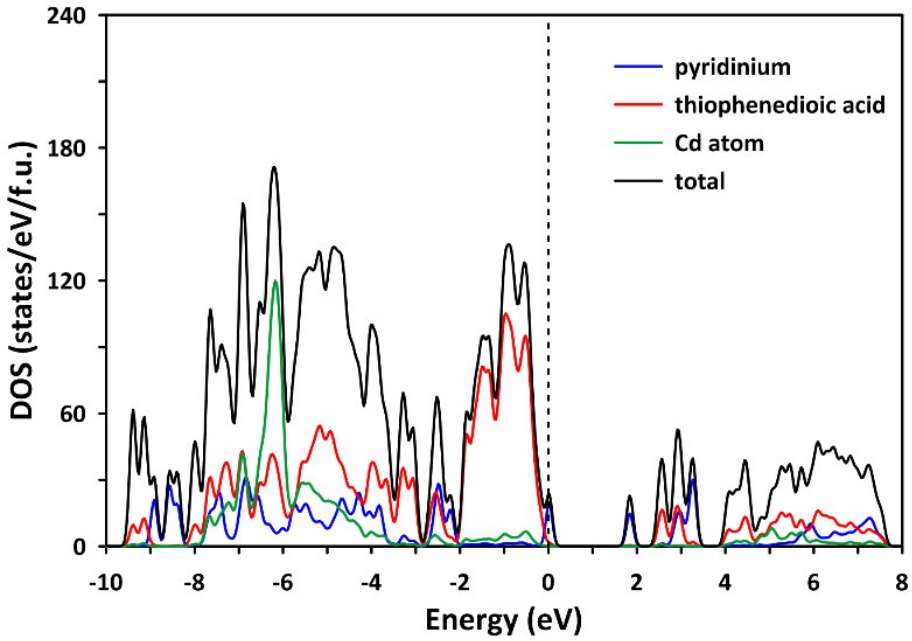

Fig. S11. Total and partial electronic density of states of compound 1.

References

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[2] J. P. Perdew, K. Burke and M. Ernzerhof, Phys. Rev. Lett., 1996, 77, 3865–3868.

[3] P. E. Blöchl, Phys. Rev. B: Condens. Matter Mater. Phys., 1994, 50, 17953–17979.

[4] G. Kresse and D. Joubert, Phys. Rev. B: Condens. Matter Mater. Phys., 1999, 59, 1758.