Supporting Information

Supramolecular isomer-dependent photochromism and emission color tuning of bipyridinium salts

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Additional characterization data and structural figures

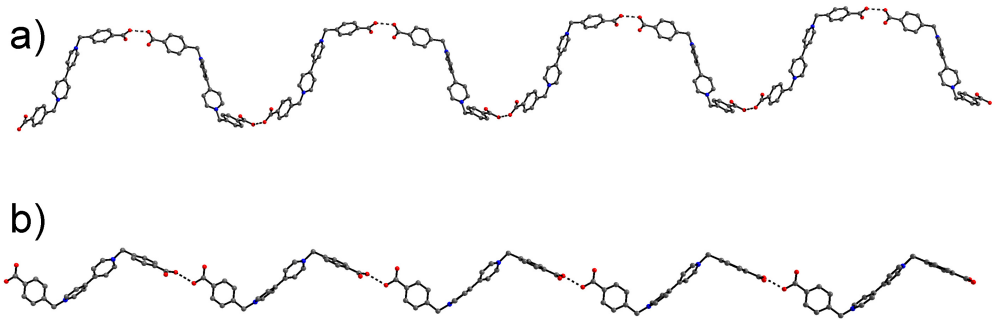

Fig. S1 a) A 1D hydrogen-bonded helical chain in **A1**. b) A 1D hydrogen-bonded zigzig chain in **A2.** The hydrogen atoms are omitted for clarity. The dashed lines represent hydrogen bonds.

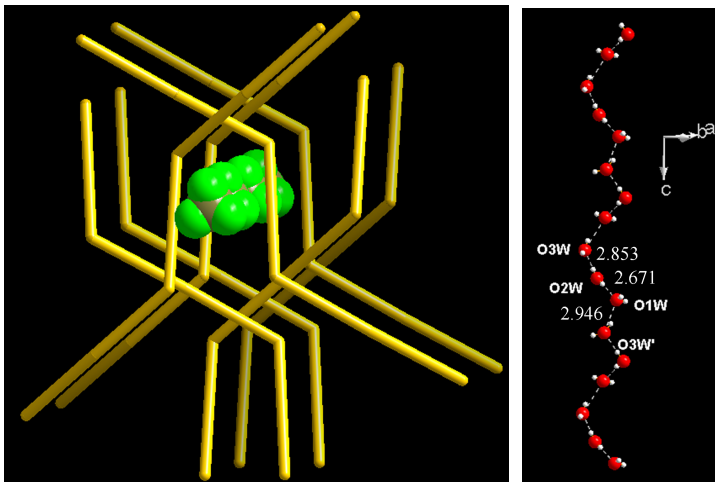

Fig. S2 Left: The topology of 1D channel in **A2.** Right: 1D meso-helical water chain confined in the channel of **A2**. The $HBpybc^+$ ligands are simplified as yellow stick. The hydrogen bond distances are in angstrom unit.

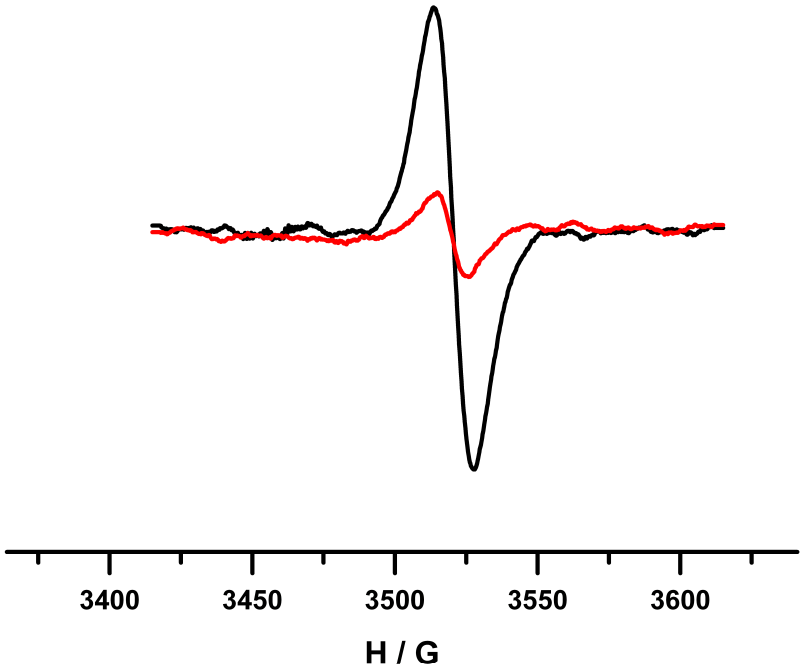

Fig. S3 The ESR spectra of A1 (black) and A2 (red) after irradiation.

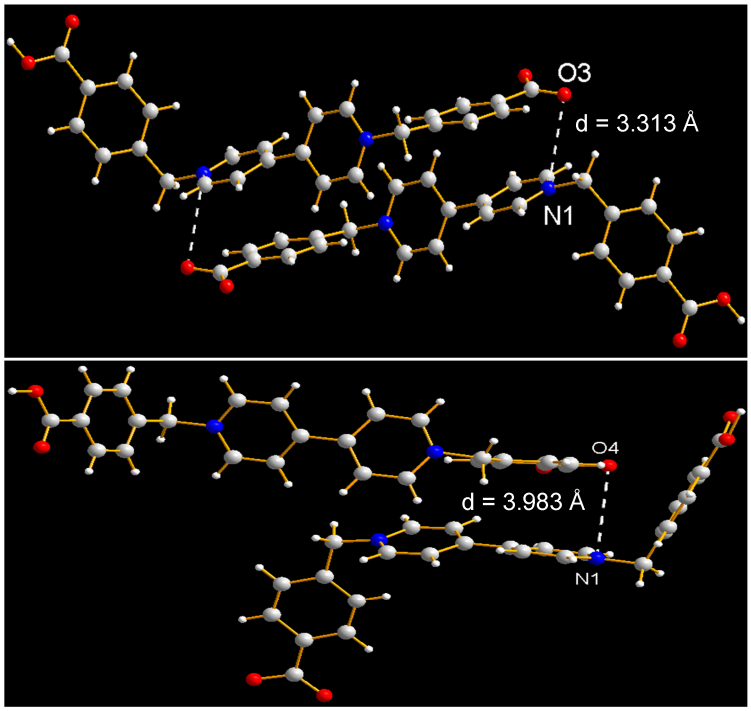

Fig. S4 The distance and orientation between the donor and acceptor in **A1** (upper) and **A2** (bottom).

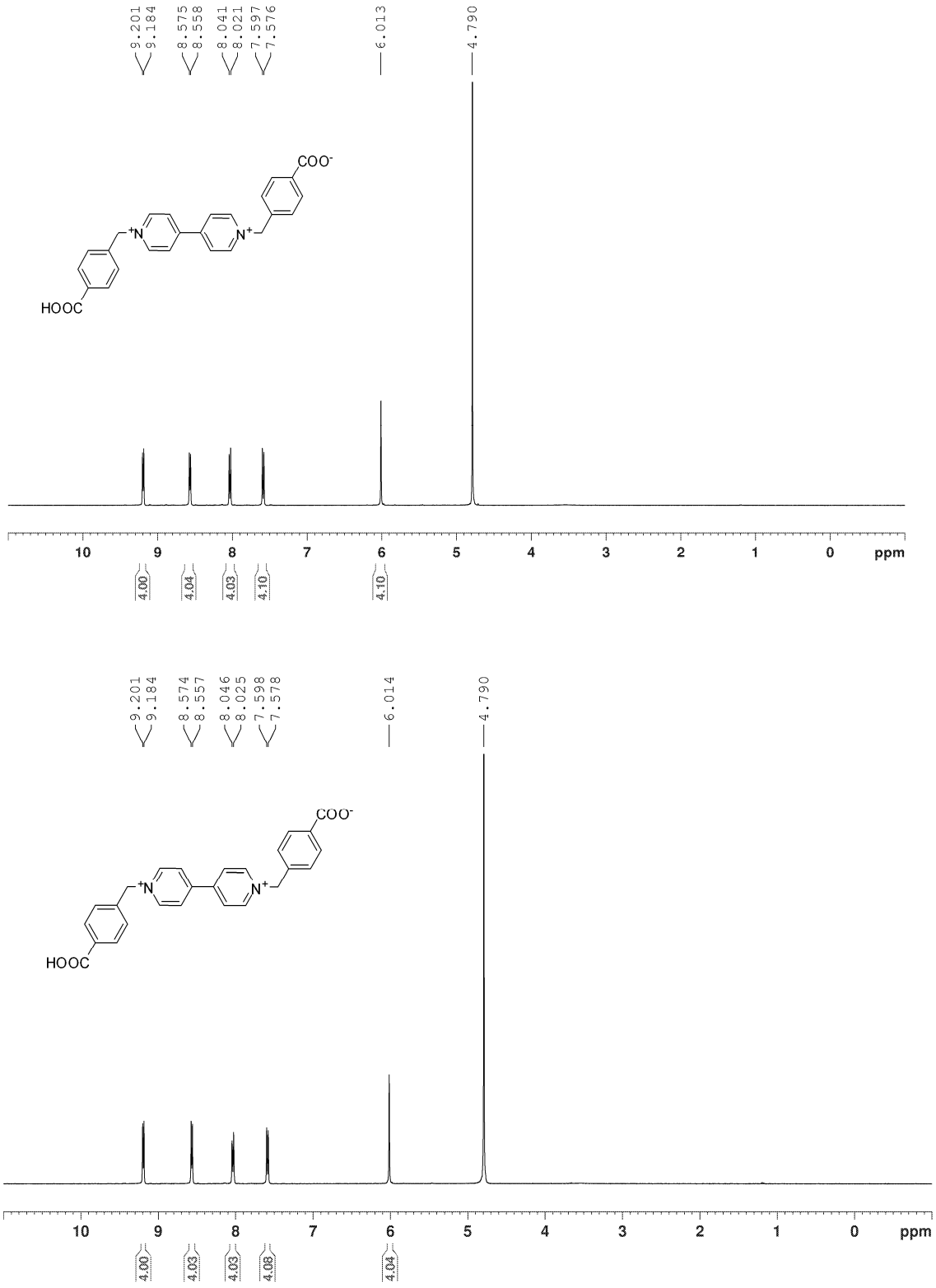

Fig. S5 ^{1}H NMR (400 MHz, D_2O) for **A1** (upper) and **A2** (bottom), respectively.

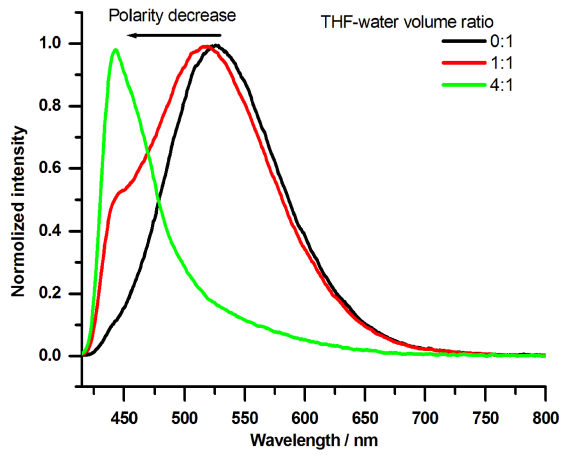

Fig. S6 Normalized fluorescence emission spectra of **A1** to show a large blue-shift of the peak position (from 524 nm to 443 nm) with decreasing solvent polarity from water (black) to THF-water (volume ratio: 4:1) mixture (green). Excitation wavelength: 360 nm.

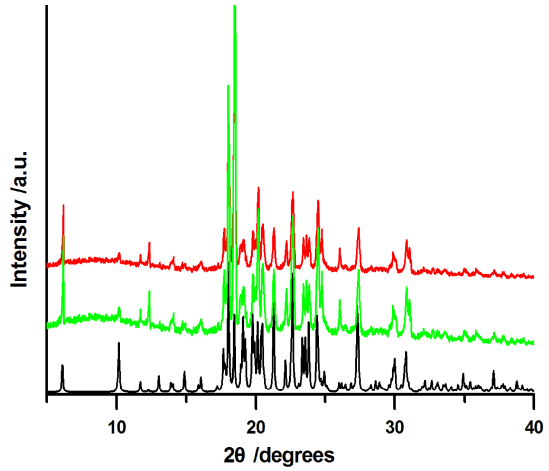

Fig. S7 Calculated XRPD pattern from the single crystal structural data of **A1** (black), experimental pattern for the colored samples of **A1** after irradiation (green), and initial sample of **A1** (red).

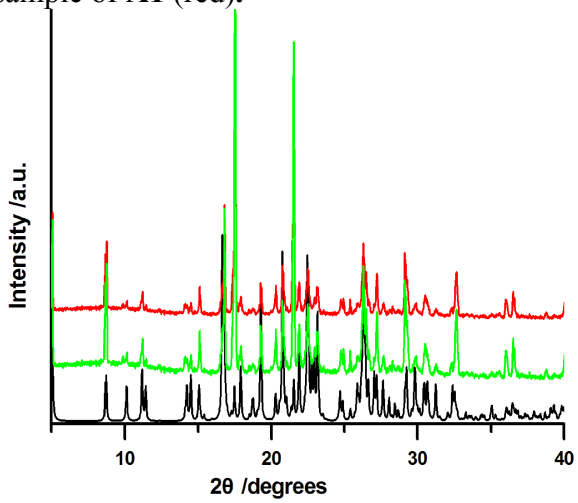

Fig. S8 Calculated XRPD pattern from the single crystal structural data of **A2** (black), experimental pattern for the colored samples of **A2** after irradiation (green), and initial sample of **A2** (red).

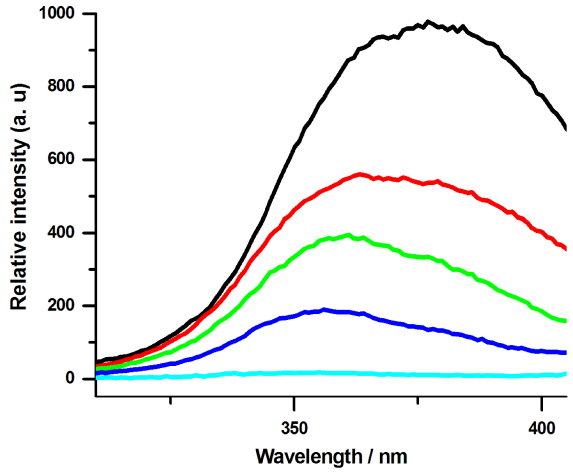

Fig. S9 Excitation spectral change of **A1** in the solid state upon irradiation with a xenon lamp.

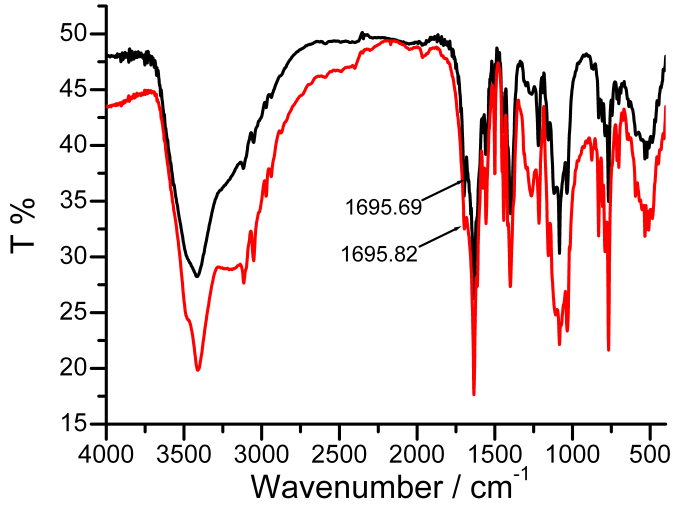

Fig. S10 IR spectra of **A1** (black) and **A2** (red). The bands appearing around 1695 cm^{-1} are attributed to the characteristic asymmetric C=O stretching vibration of the carboxylic group in monoprotonated $HBpybc^{+}$.