Supporting Information

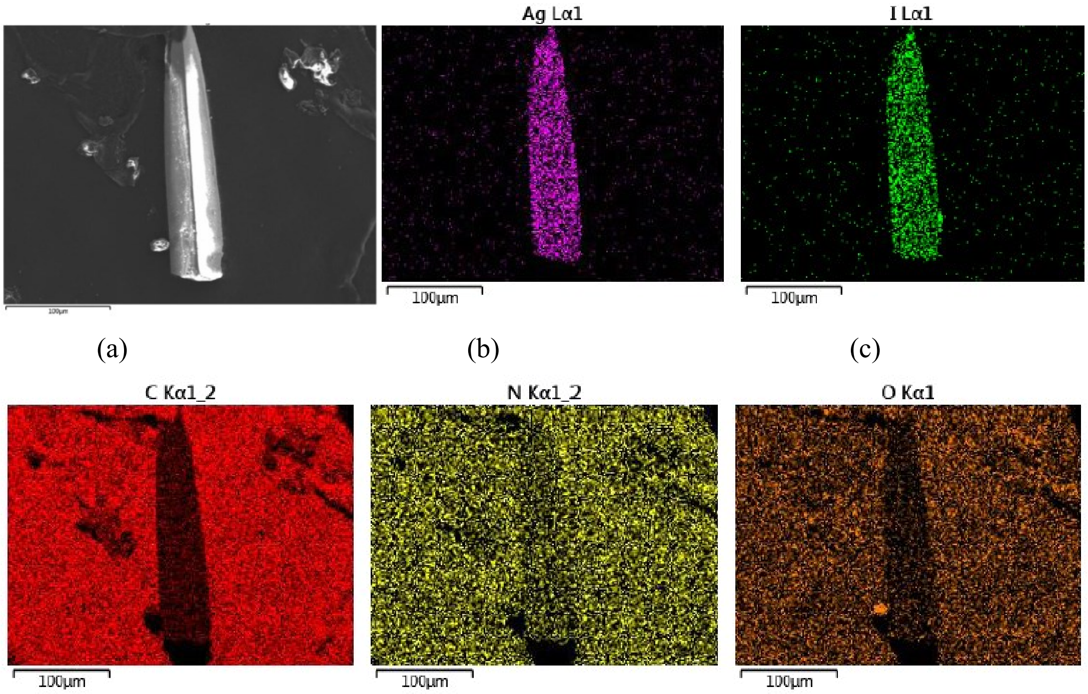
A unique formyl iodoargentate exhibiting luminescent and photocurrent response properties

Lili Yang,[a] Jian Zhou,*[a] Litao An,[b] Shumei Cao,*[a] and Jun Hu[a]

General Remarks. All analytical grade chemicals were obtained commercially and used without further purification. IR spectra were obtained from a powdered sample pelletized with KBr on an ABB Bomen MB 102 series IR spectrophotometer in the range of 200–1200cm^{-1}. Energy-dispersive X-ray analysis (EDXA) was taken by using a JEOL JSM-6700F field-emission scanning electron microscope. Room-temperature optical diffuse reflectance spectra of the powdered samples were obtained with a Shimadzu UV-3150 spectrometer. The absorption data were calculated from reflectance spectra by using the Kubelka–Munk function: $a/S = (1-R^2)/2R$, where a is the absorption coefficient, S is the scattering coefficient, and R is the reflectance. PXRD patterns were obtained using a Bruker D8 Advance XRD diffractometer with Cu Kα radiation (λ = 1.54056 Å).The crystals of **1** were grinded and pressed uniformly on the FTO glass. The photocurrent experiment was performed on a CHI650E electrochemistry work station in a three-electrode system, the sample coated ITO glass as the working electrode, a Pt slice as auxiliary electrode and a saturated calomel electrode (SCE) as reference electrode. The supporting electrolyte solution was 0.1 mol·dm^{-3} Na_2SO_4 aqueous solution (100 mL). A 500 W Xe lamp with 420 nm was used as the illumination source. The lamp was kept on continuously, and a manual shutter was used to block exposure of the sample to the light. The sample was typically irradiated at intervals of 50 s.

Crystal Structure Determination

Single-crystal X-ray diffraction data for **1** were recorded on a Bruker APEX-II CCD diffractometer using a ω-scan method with graphite monochromated Mo Kα radiation (λ = 0.71073 Å) at 296(2) K to a maximum 2θ value (55.64 °). Absorption corrections were applied were applied using SADABS. The structure of **1** was solved by Direct Methods and refined by full-matrix least-squares techniques using the SHELXL-2018/3 program. Non-hydrogen atoms were refined with anisotropic displacement parameters. The H atoms bonded to C/N atoms were positioned with idealized geometry and refined with fixed isotropic displacement parameters.



(a) (b) (c)

(d) (e) (f)

Fig. S1 (a) SEM image of **1**. (b-f) EDS elemental mappings of Ag, I, C, N and Ofor **1**.

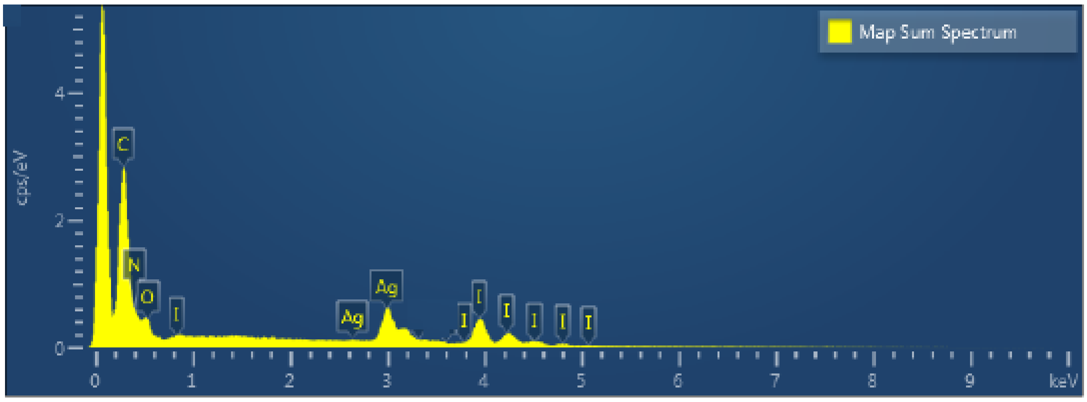


Fig. S2 EDS spectrum of **1**.

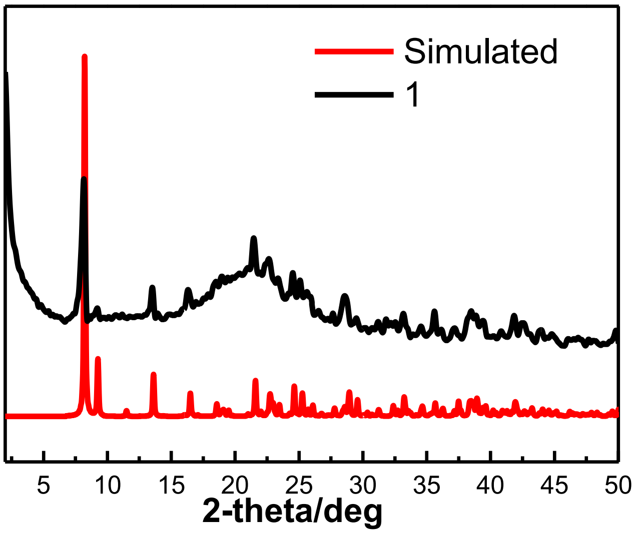


Fig. S3 Simulated and experimental powder XRD patterns of **1**.

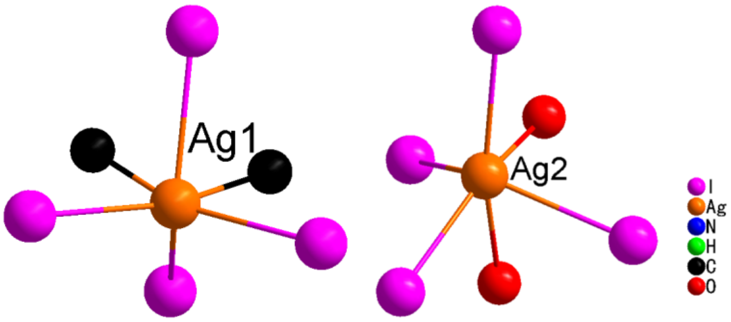


Fig. S4 the coordination environments of Ag^+ ions.

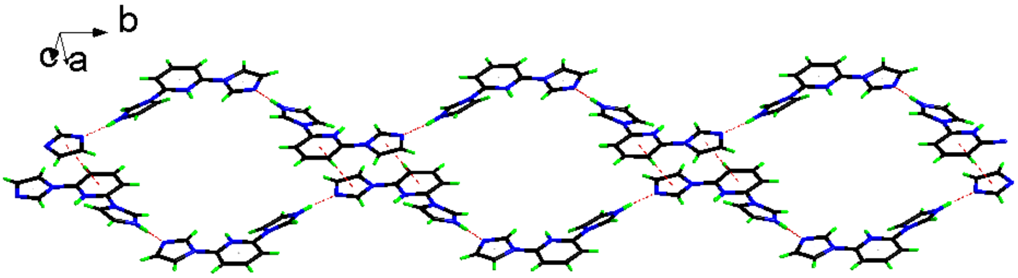


Fig. S5 The π-π stacking interactions between 1-D $[H_2L^{2+}]_n$ H-bond chains.

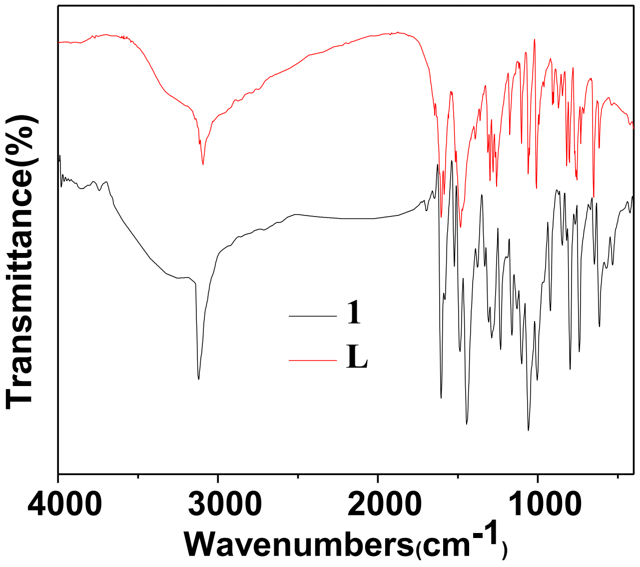


Fig. S6 The IR spectra of **1** and L.

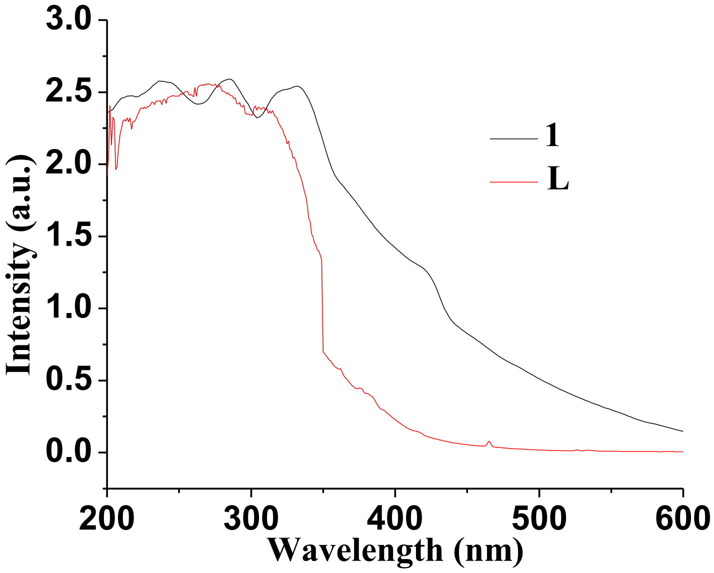


Fig. S7 The excitation spectra of L and **1**.

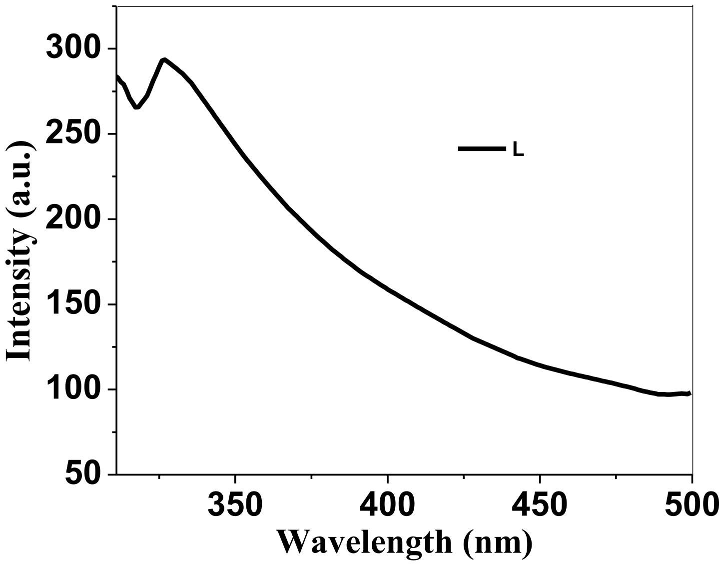


Fig. S8 Emission spectrum of L at room temperature.