Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information (SI)

Two Photochromic Methylated Nicotinohydrazide Iodoargentate Hybrids

Junju Shen, Feng Wang, Xiangxia Li, Tanlai Yu, Pengfei Hao and Yunlong Fu*

School of Chemistry & Material Science, Shanxi Normal University, Linfen 041004, P. R. China

Fax & Tel: +86 357 2053716; E-mail: yunlongfu@sxnu.edu.cn

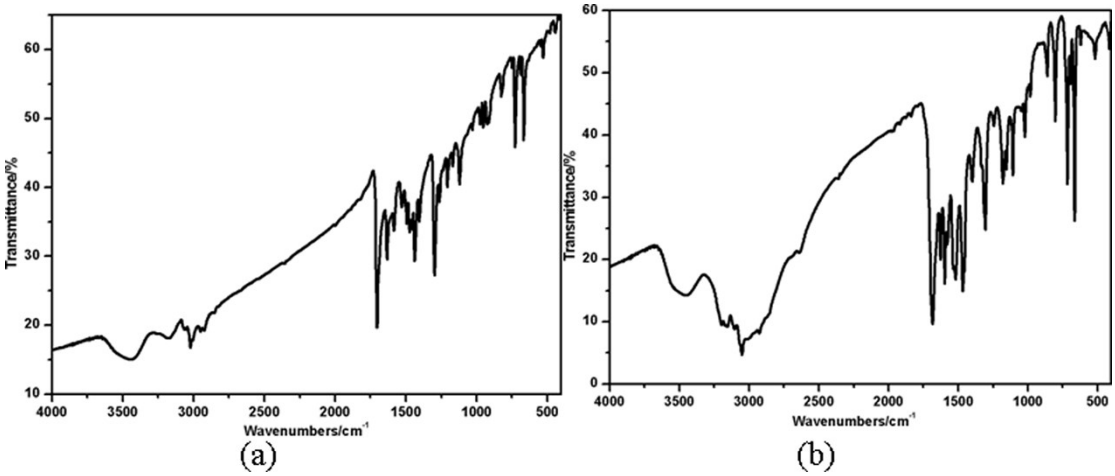


Fig. S1 FT-IR spectra of **1** (a) and **2** (b).

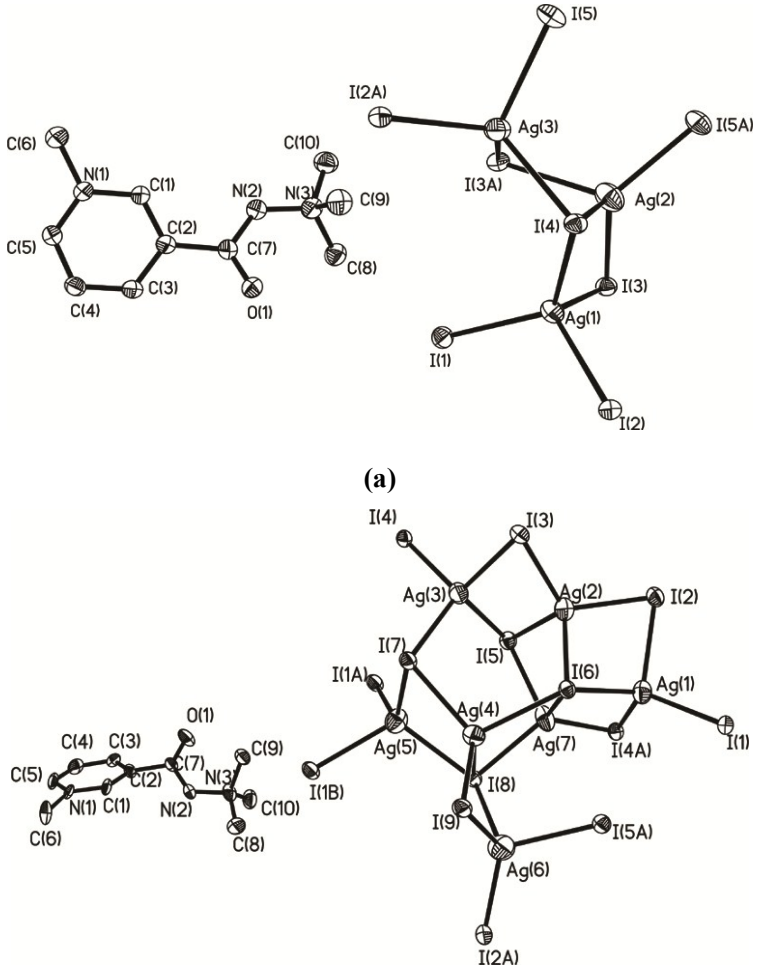


Fig. S2 The structure unit diagrams of **1** (a) and **2** (b). The disordered Ag atoms in **1** are omitted for clarity.

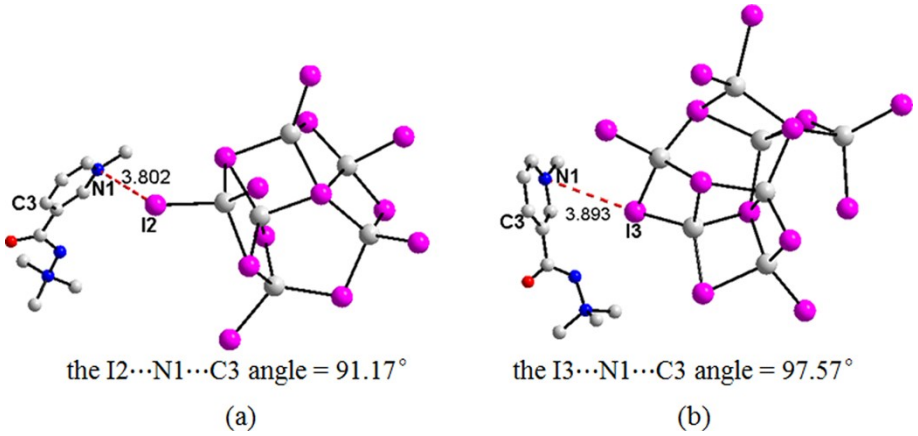
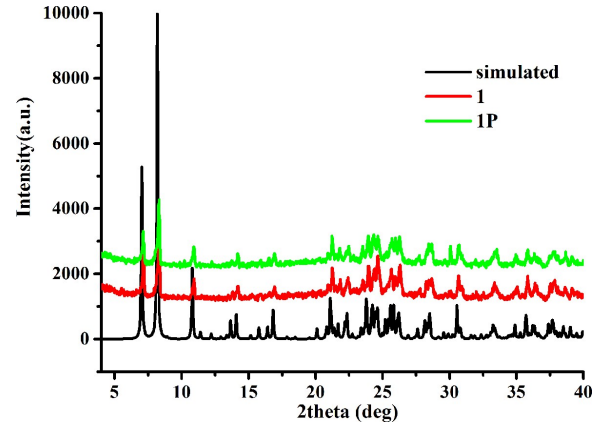
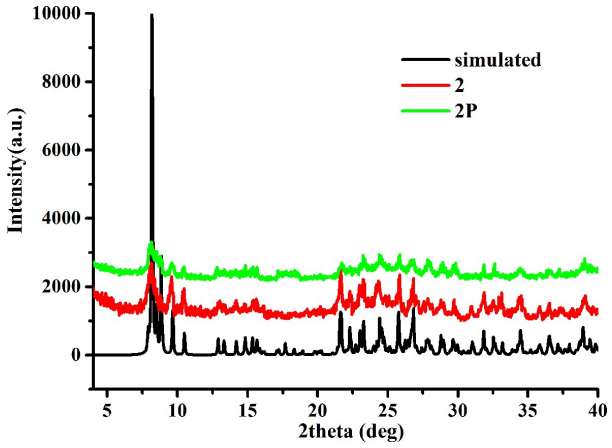


Fig. S3 The shortest distance and orientation between the acceptor (N atom of pyridinium ring of MNH^{2+} cation) and donor (I atom of iodoargentate anions) in **1** (a) and **2** (b). Distances are in angstrom (Å).



(a)



(b)

Fig. S4 The PXRD patterns of **1** (a) and **2** (b) before and after irradiation.

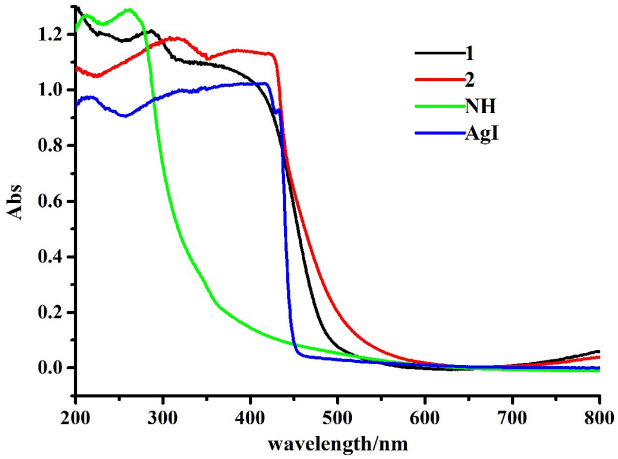
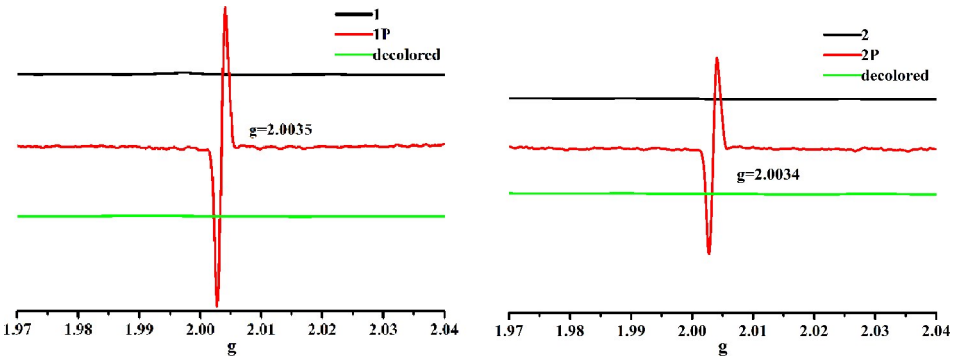


Fig. S5 UV−vis absorption spectra of starting materials, **1** and **2** before irradiation.



(a) **(b)**

Fig. S6 EPR spectra of **1** (a) and **2** (b).

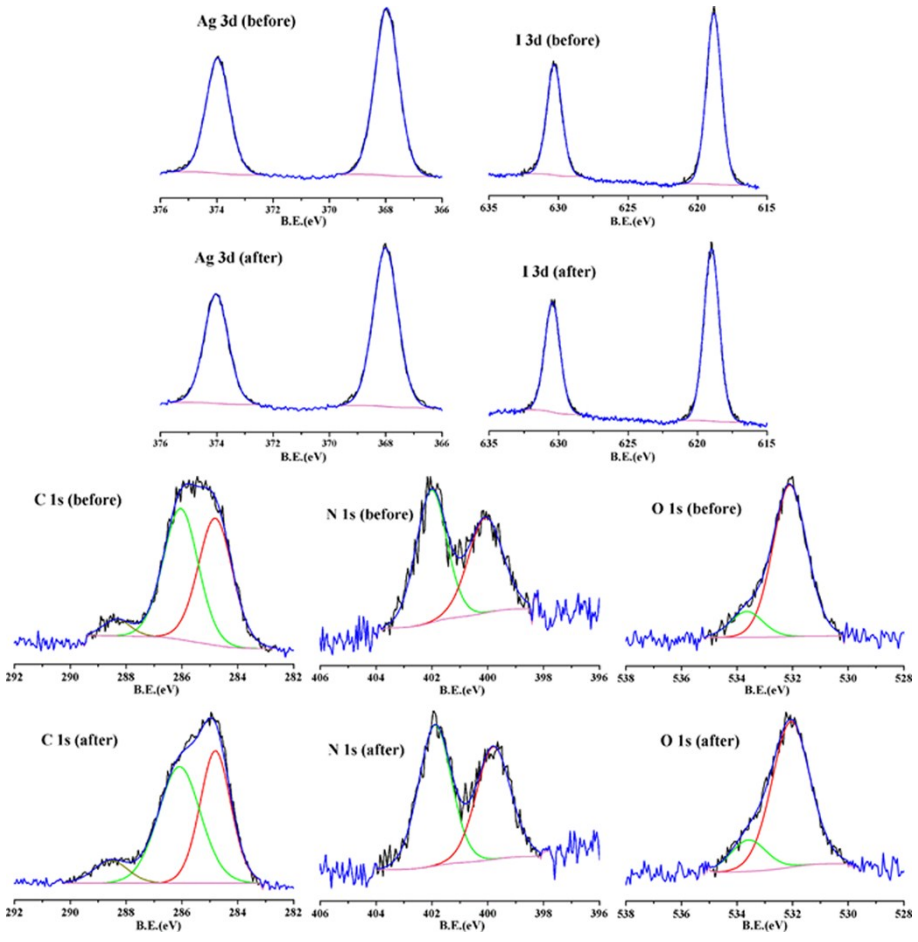


Fig. S7 XPS core-level spectra of **1** before and after irradiation.

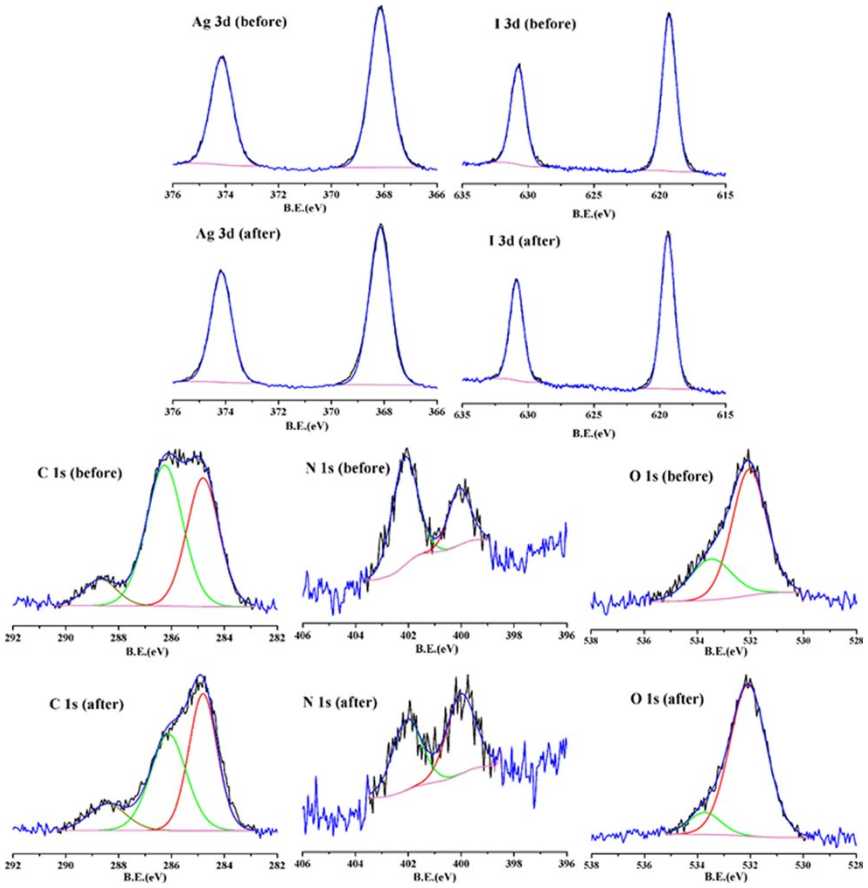


Fig. S8 XPS core-level spectra of **2** before and after irradiation.

Table S1. Selected bond lengths [Å] and angles [°] for **1** and **2**

Compound **1**			
Ag(1)-I(1)	2.7908(16)	Ag(2)-I(3)#1	2.935(2)
Ag(1)-I(2)	2.8762(17)	Ag(3)-I(2)#4	2.8042(18)
Ag(1)-I(3)	2.8876(17)	Ag(3)-I(4)	2.8688(17)
Ag(1)-I(4)	2.9074(15)	Ag(3)-I(5)	2.8847(17)
Ag(2)-I(5)#2	2.793(2)	Ag(3)-I(3)#1	2.9774(17)
Ag(2)-I(4)	2.833(2)	Ag(3)-Ag(2)#1	2.997(2)
Ag(2)-I(3)	2.907(2)		
I(1)-Ag(1)-I(2)	109.95(5)	I(5)#2-Ag(2)-I(3)#1	115.92(8)
I(1)-Ag(1)-I(3)	104.51(5)	I(4)-Ag(2)-I(3)#1	95.18(6)
I(2)-Ag(1)-I(3)	110.61(5)	I(3)-Ag(2)-I(3)#1	93.41(6)
I(1)-Ag(1)-I(4)	120.98(5)	I(2)#4-Ag(3)-I(4)	120.21(6)
I(2)-Ag(1)-I(4)	99.33(5)	I(2)#4-Ag(3)-I(5)	102.72(5)
I(3)-Ag(1)-I(4)	111.38(5)	I(4)-Ag(3)-I(5)	113.25(6)
I(5)#2-Ag(2)-I(4)	117.29(7)	I(2)#4-Ag(3)-I(3)#1	115.24(6)
I(5)#2-Ag(2)-I(3)	117.36(7)	I(4)-Ag(3)-I(3)#1	93.51(5)
I(4)-Ag(2)-I(3)	113.01(7)	I(5)-Ag(3)-I(3)#1	112.33(5)
Compound **2**			
Ag(1)-I(1)	2.7760(9)	Ag(5)-I(7)	2.8562(11)
Ag(1)-I(4)#1	2.8546(10)	Ag(5)-I(1) #3	2.9647(10)
Ag(1)-I(2)	2.8602(10)	Ag(6)- I(9)	2.7634(11)
Ag(1)-I(6)	3.0209(10)	Ag(6)-I(2)#1	2.8115(12)
Ag(2)-I(3)	2.7807(10)	Ag(6)-I(5)#1	2.9573(12)
Ag(2)-I(2)	2.7930(10)	Ag(6)-I(8)	3.1233(11)
Ag(2)-I(6)	2.9199(9)	Ag(7)- I(4)#1	2.8463(9)
Ag(2)-I(5)	2.9551(10)	Ag(7)-I(5)	2.9009(11)
Ag(3)-I(3)	2.8118(10)	Ag(7)-I(8)	2.8081(10)
Ag(3)-I(7)	2.8171(9)	Ag(7)- I(6)	2.9520(10)
Ag(3)-I(4)	2.8254(9)	Ag(1)-Ag(2)	3.3284(11)
Ag(3)-I(5)	2.9058(9)	Ag(1)-Ag(7)	3.0051(11)
Ag(4)-I(9)	2.7948(9)	Ag(2)-Ag(3)	3.1249(11)
Ag(4)-I(7)	2.8516(9)	Ag(2)-Ag(6)#2	3.1255(12)
Ag(4)-I(8)	2.9308(9)	Ag(4)-Ag(5)	3.3170(11)
Ag(4)-I(6)	2.9659(9)	Ag(4)-Ag(6)	3.3277(12)
Ag(5)-I(8)	2.8994(10)	Ag(6)-Ag(2)#1	3.1255(12)
Ag(5)-I(1)#2	2.8266(10)		
I(1)-Ag(1)-I(4)#1	117.50(3)	I(9)-Ag(4)-I(6)	107.16(3)
I(1)-Ag(1)-I(2)	107.03(3)	I(7)-Ag(4)-I(6)	105.07(3)
I(4)#1-Ag(1)-I(2)	107.91(3)	I(8)-Ag(4)-I(6)	110.61(3)
I(1)-Ag(1)-I(6)	106.16(3)	I(8)-Ag(5)-I(1)#3	112.87(3)

I(4)#1-Ag(1)-I(6)	116.12(3)	I(1)#2-Ag(5)-I(7)	117.73(3)
I(2)-Ag(1)-I(6)	100.46(3)	I(1)#2-Ag(5)-I(8)	112.80(3)
I(3)-Ag(2)-I(2)	117.89(3)	I(7)-Ag(5)-I(8)	108.42(3)
I(3)-Ag(2)-I(6)	108.44(3)	I(1)#2-Ag(5)-I(1)#3	90.31(3)
I(2)-Ag(2)-I(6)	104.63(3)	I(7)-Ag(5)-I(1)#3	113.92(3)
I(3)-Ag(2)-I(5)	109.04(3)	I(9)-Ag(6)-I(2)#1	126.98(4)
I(2)-Ag(2)-I(5)	111.51(3)	I(9)-Ag(6)-I(5)#1	110.72(4)
I(6)-Ag(2)-I(5)	104.35(3)	I(2)#1-Ag(6)-I(5)#1	110.91(4)
I(3)-Ag(3)-I(7)	116.56(3)	I(9)-Ag(6)-I(8)	103.05(3)
I(3)-Ag(3)-I(4)	107.95(3)	I(2)#1-Ag(6)-I(8)	106.25(4)
I(7)-Ag(3)-I(4)	113.53(3)	I(5)#1-Ag(6)-I(8)	92.73(3)
I(3)-Ag(3)-I(5)	109.58(3)	I(8)-Ag(7)-I(4)#1	115.36(3)
I(7)-Ag(3)-I(5)	106.66(3)	I(8)-Ag(7)-I(5)	101.40(3)
I(4)-Ag(3)-I(5)	101.45(3)	I(4)#1-Ag(7)-I(5)	97.82(3)
I(9)-Ag(4)-I(7)	118.88(3)	I(8)-Ag(7)-I(6)	114.62(3)
I(9)-Ag(4)-I(8)	107.36(3)	I(4)#1-Ag(7)-I(6)	118.63(3)
I(7)-Ag(4)-I(8)	107.68(3)	I(5)-Ag(7)-I(6)	104.91(3)

Symmetry code: for **1**: #1 x,-y+1/2,z+1/2; #2 x,-y+1/2,z-1/2; #4 x,y,z+1; for **2**: #1 -x+1/2,y-1/2,-z+1/2; #2 -x+1/2,y+1/2,-z+1/2; #3 x+1/2,-y+1/2,z+1/2.