Stoichiometry-controlled structural and functional variation in two photochromic iodoargentates with fast and wide range response

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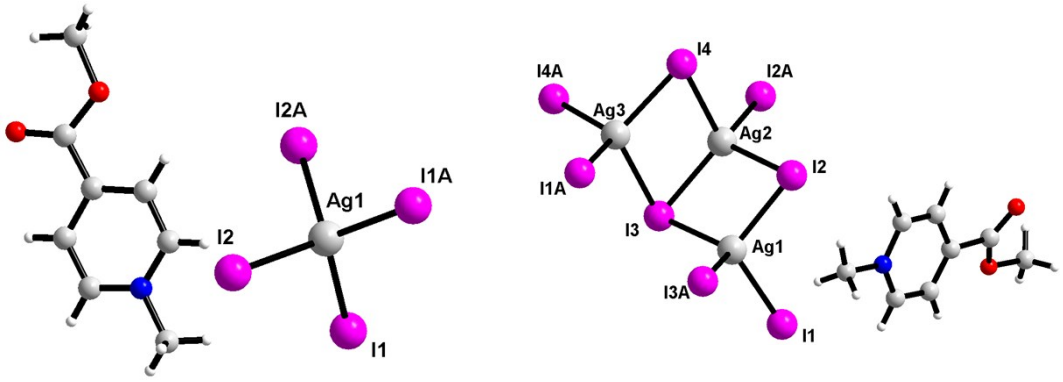
Supporting Information (SI)

Supporting Information of two compounds: The asymmetric unit diagram of **1** and **2** (Fig. S1), Topological network of **2** (Fig. S2), Infrared Spectroscopy (Fig. S3), X–ray powder diffraction (XRPD) patterns (Fig. S4) and Selected bond lengths (Å) and angles (°) for **1** and **2** (Tables S1), Optical absorption comparison of **1**, **2** and $[MV][Ag_2I_4]$ (Tables S2).



(a) (b)

Fig. S1 The asymmetric unit diagram of **1** (a) and **2** (b).

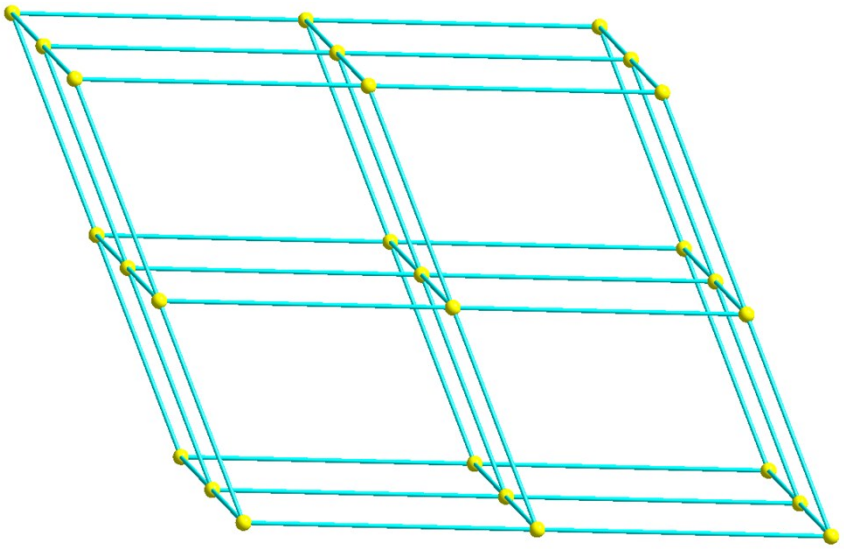


Fig. S2 View of the pcu topological network in the compound **2**.

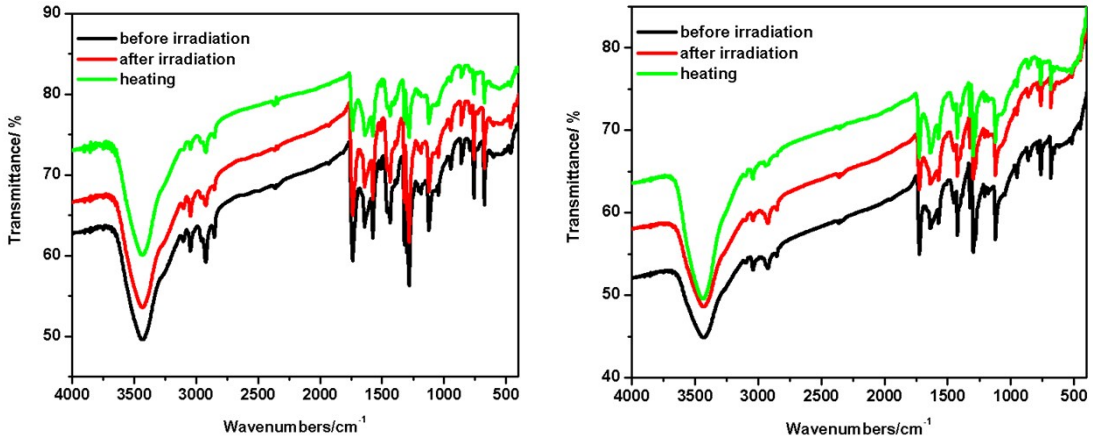


Fig. S3 IR spectra of **1** and **2.**

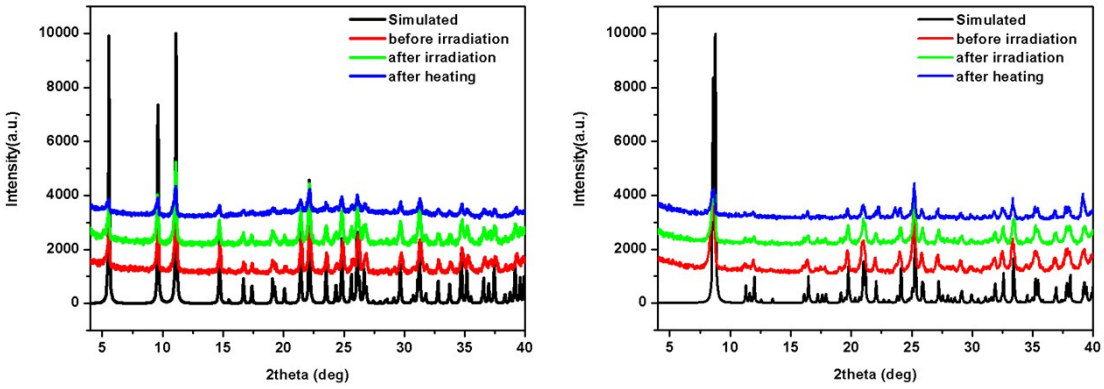


Fig. S4 X-ray powder diffraction (XRPD) patterns of **1** and **2**.

Table S1 Selected bond lengths (Å) and angles (°) for **1** and **2** at 293(2) K

Compound **1**			
Ag(1)-I(1)	2.8245(13)	Ag(1)-I(2)#1	2.9056(12)
Ag(1)-I(1)#1	2.8351(13)	Ag(1)-I(2)	2.9085(12)
I(1)-Ag(1)-I(1)#1	116.36(5)	I(1)-Ag(1)-I(2)	106.91(4)
I(1)-Ag(1)-I(2)#1	108.54(4)	I(1)#1-Ag(1)-I(2)	105.48(4)
I(1)#1-Ag(1)-I(2)#1	106.70(4)	I(2)#1-Ag(1)-I(2)	113.00(4)
Compound **2**			
Ag(1)-I(1)	2.7739(14)	Ag(1)-I(3)#1	3.0173(15)
Ag(1)-I(3)	2.8528(13)	Ag(1)-Ag(1)#1	3.169(2)
Ag(1)-I(2)	2.8563(14)	Ag(2)-I(4)	2.8631(14)
Ag(2)-I(2)	2.8766(14)	Ag(2)-I(2)#2	2.8637(14)
Ag(2)-I(3)	2.8807(14)	Ag(3)-I(4)	2.8530(15)
Ag(3)-I(1)#1	2.7652(15)	Ag(3)-I(3)	3.0097(16)
Ag(3)-I(4)#3	2.8444(14)	Ag(2)-Ag(2)#2	3.161(2)
Ag(1)-Ag(2)	3.3477(16)	Ag(2)-Ag(3)	3.2135(18)
I(1)-Ag(1)-I(3)	117.58(5)	I(1)-Ag(1)-I(3)#1	102.71(4)

I(1)-Ag(1)-I(2)	110.82(5)	I(3)-Ag(1)-I(3)#1	114.72(4)
I(3)-Ag(1)-I(2)	109.10(4)	I(2)-Ag(1)-I(3)#1	100.52(4)
I(4)-Ag(2)-I(2)#2	99.52(4)	I(4)-Ag(2)-I(3)	114.53(4)
I(4)-Ag(2)-I(2)	105.56(4)	I(2)#2-Ag(2)-I(3)	116.57(5)
I(2)#2-Ag(2)-I(2)	112.33(4)	I(2)-Ag(2)-I(3)	107.76(4)
I(1)#1-Ag(3)-I(4)#3	118.72(5)	I(1)#1-Ag(3)-I(3)	103.11(4)
I(1)#1-Ag(3)-I(4)	113.89(5)	I(4)#3-Ag(3)-I(3)	103.79(4)
I(4)#3-Ag(3)-I(4)	105.83(4)	I(4)-Ag(3)-I(3)	110.97(5)

Symmetry code:

For 1: #1 -x+y,y,z-1/2; #2 -x+y,y,z+1/2. For 2: #1 -x+1/2,-y+1/2,-z+1; #2 -x,y,-z+1/2; #3 -x,-y+1,-z+1.

Table S2 Optical absorption comparison of **1**, **2** and [MV][Ag_2I_4].

Compounds	**Inorganic moiety**	**Color**	**visible absorption band edges**	**Intermolecular Charge transfer**	**photo-induced electron transfer**	**Photo-chromism**
[MV][Ag_2I_4]	$(Ag_2I_4)^{2-}$ chain	Red	610 nm	Strong	No	No
[MCMP][AgI_2] (1)	$(Ag_2I_4)^{2-}$ chain	Dark yellow	540 nm	Weak	Yes	Yes
[MCMP][Ag_3I_4] (2)	$(Ag_3I_4)^{-}$ framework	Pale yellow	492 nm	Weak	Yes	Yes