Electronic Supporting Information (ESI) for

A new metal complex-templated silver iodobismuthate exhibiting photocurrent response and photocatalytic property

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1. More structural details

Table S1 Selected bond lengths (Å) and bond angles (°) for compound **1**.

Bi(1)−I(1)#1	3.0636(5)	I(2)−I(4)#6	0.522(18)
Bi(1)−I(1)#2	3.0636(5)	I(2)−I(3)	2.85(2)
Bi(1)−I(1)#3	3.0637(5)	I(3)−I(3)#6	0.39(3)
Bi(1)−I(1)#4	3.0638(5)	I(3)−I(4)#6	2.53(3)
Bi(1)−I(1)#5	3.0637(5)	I(3)−I(4)	2.82(3)
Bi(1)−I(1)	3.0637(5)	Zn(1)−N(1)#7	2.128(5)
Ag(1)−I(2B)	2.653(12)	Zn(1)−N(1)	2.128(5)
Ag(1)−I(1)	2.814(2)	Zn(1)−N(1)#8	2.128(5)
Ag(1)−I(2)	2.958(11)	Zn(1)−N(2)#8	2.150(5)
Ag(1)−I(1)#3	3.069(2)	Zn(1)−N(2)	2.150(5)
Ag(1)−I(1)#2	3.133(2)	Zn(1)−N(2)#7	2.150(5)
I(1)#1−Bi(1)−I(1)#2	180.0	Ag(1)#2−I(1)−Ag(1)#3	135.16(7)
I(1)#1−Bi(1)−I(1)#3	89.630(14)	I(1)#2−Bi(1)−I(1)#5	89.631(14)
I(1)#2−Bi(1)−I(1)#3	90.370(14)	I(1)#3−Bi(1)−I(1)#5	180.0
I(1)#1−Bi(1)−I(1)#4	89.631(14)	I(1)#4−Bi(1)−I(1)#5	89.633(14)
I(1)#2−Bi(1)−I(1)#4	90.367(14)	I(1)#1−Bi(1)−I(1)	90.368(14)
I(1)#3−Bi(1)−I(1)#4	90.365(14)	I(1)#2−Bi(1)−I(1)	89.634(14)
I(1)#1−Bi(1)−I(1)#5	90.370(14)	I(1)#3−Bi(1)−I(1)	89.634(14)
I(1)#4−Bi(1)−I(1)	180.0	N(1)#7−Zn(1)−N(1)	95.6(2)
I(1)#5−Bi(1)−I(1)	90.368(14)	N(1)#7−Zn(1)−N(1)#8	95.6(2)
I(2B)−Ag(1)−I(1)	124.4(3)	N(1)−Zn(1)−N(1)#8	95.6(2)
I(1)−Ag(1)−I(2)	120.4(2)	N(1)#7−Zn(1)−N(2)#8	167.65(19)
I(2B)−Ag(1)−I(1)#3	123.0(3)	N(1)−Zn(1)−N(2)#8	94.82(19)
I(1)−Ag(1)−I(1)#3	94.37(6)	N(1)#8−Zn(1)−N(2)#8	76.8(2)
I(2)−Ag(1)−I(1)#3	124.8(3)	N(1)#7−Zn(1)−N(2)	94.8(2)

I(1)−Ag(1)−I(1)#2	92.99(6)	N(1)−Zn(1)−N(2)	76.8(2)
I(2)−Ag(1)−I(1)#2	126.1(3)	N(1)#8−Zn(1)−N(2)	167.65(19)
I(1)#3−Ag(1)−I(1)#2	88.98(5)	N(2)#8−Zn(1)−N(2)	94.02(19)
Ag(1)−I(1)−Bi(1)	71.53(4)	N(1)#7−Zn(1)−N(2)#7	76.8(2)
Ag(1)−I(1)−Ag(1)#2	80.51(4)	N(1)−Zn(1)−N(2)#7	167.65(19)
Bi(1)−I(1)−Ag(1)#2	68.26(4)	N(1)#8−Zn(1)−-N(2)#7	94.83(19)
Ag(1)−I(1)−Ag(1)#3	79.40(4)	N(2)#8−Zn(1)−N(2)#7	94.02(19)
Bi(1)−I(1)−Ag(1)#3	67.45(4)	N(2)−Zn(1)−N(2)#7	94.02(19)

Symmetry transformations used to generate equivalent atoms: #1 −*x*+*y*+1, −*x*+1, *z*; #2 *x*−*y*+1/3, *x*−1/3, −*z*+5/3; #3 *y*+1/3, −*x*+*y*+2/3, −*z*+5/3; #4 −*x*+4/3, −*y*+2/3, −*z*+5/3; #5 −*y*+1, *x*−*y*, *z*; #6 −*x*+4/3, −*y*+5/3, −*z*+5/3; #7 −*x*+*y*+1, −*x*+2, *z*; #8 −*y*+2, *x*−*y*+1, *z*.

Table S2 Hydrogen bonds (Å) and angles (º) for compound **1**.

C−H···I	d(C−H)	d(H···I)	d(C···I)	<(CHI)
C(4)−H(4)···I(1)#3	0.93	3.14	3.857(7)	135.9
C(7)−H(7)···I(1)	0.93	3.33	3.983(7)	129.6
C(2)−H(2)···I(2B)#9	0.93	3.15	3.782(15)	126.6
C(9)−H(9)···I(2B)#10	0.93	3.31	3.976(14)	130.4

Symmetry transformations used to generate equivalent atoms: #3 *y*+1/3, −*x*+*y*+2/3, −*z*+5/3; #9 −*x*+5/3, −*y*+4/3, −*z*+4/3; #10 −*x*+*y*+2/3, −*x*+4/3, *z*+1/3.

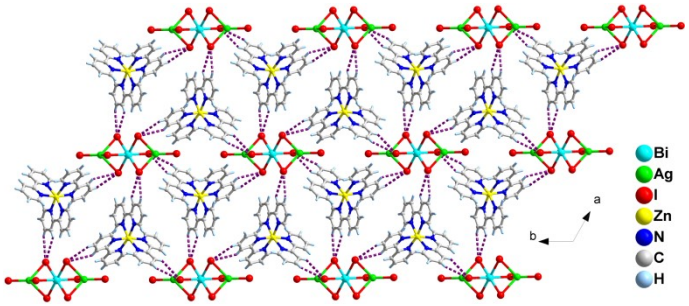

Fig. S1 View of the discrete $[Ag_2BiI_6(I)]_n^{2n-}$ anions along the *c* axis; dashed lines show the C−H···I interactions.

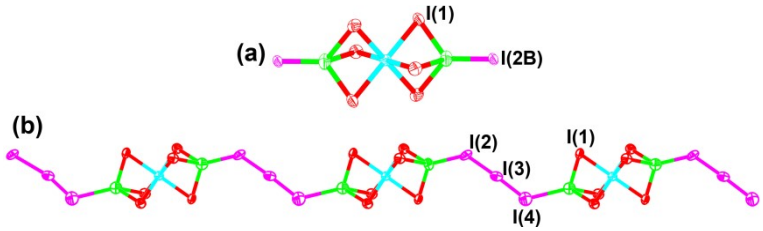

Fig. S2 (a) The discrete $[Ag_2BiI_6(I)]_n^{2n-}$ moiety. (b) The 1D $[Ag_2BiI_6(I_3)]_n^{2n-}$ chain. Thermal ellipsoids are at 50% probability.

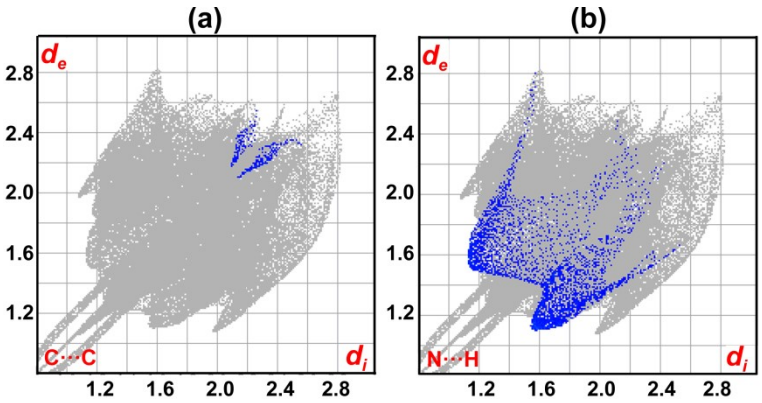

Fig. S3 (a) The C···C interaction. (b) The N···H interaction.

2. Physical measurements

2a). EDX

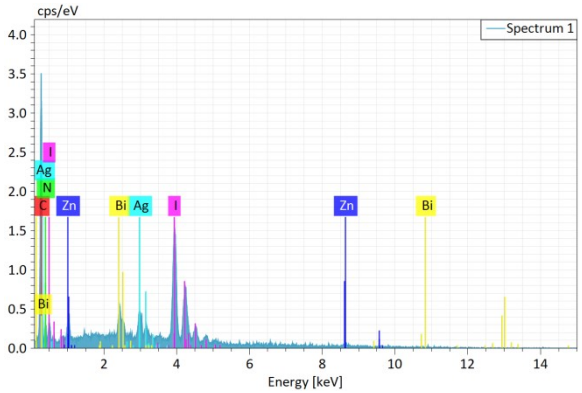

Fig. S4 EDX spectrum of compound **1**.

2b). TGA

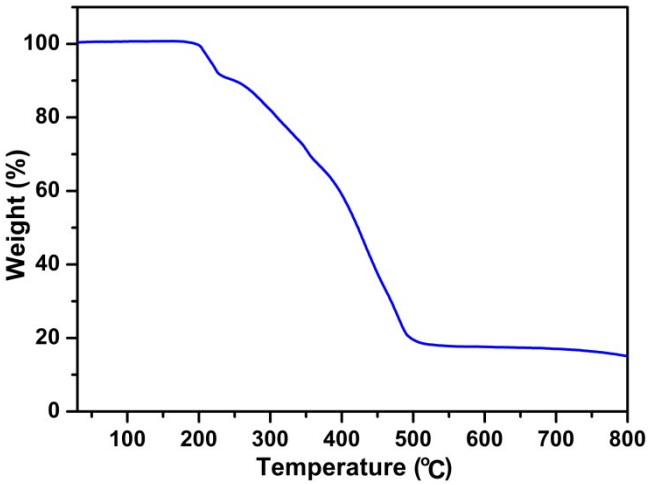

Fig. S5 The TGA curve of compound **1**.

2c). UV-vis

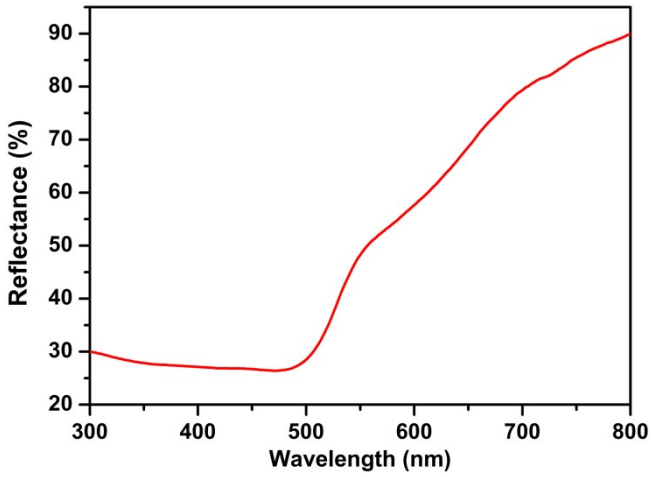

Fig. S6 The UV-Vis diffuse reflectance spectrum of compound **1**.

2d). Photocatalysis

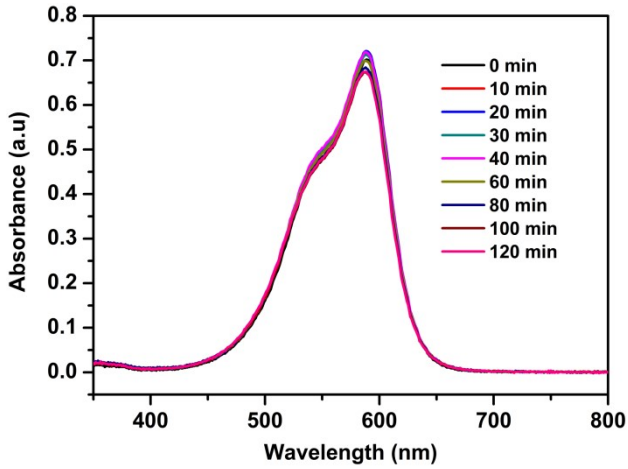

Fig. S7 The blank experiment of compound **1**.

3. DFT calculations

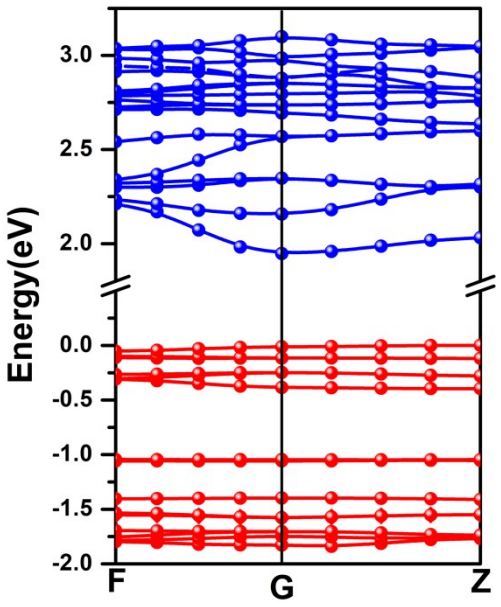

Fig. S8 The band structure of compound **1**. The VB maximum is set at 0 eV (dashed line).