Comparison Studies of Hybrid Lead Halide $[MPb_2X_7]^{2-}$ (M = Cu, Ag; X = Br, I) Chains: Band Structures and Visible Light Driven Photocatalytic Properties

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Supporting Information

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

Pb(1)-I(1)	2.9448(6)	Pb(2)-I(2)	3.0611(6)
Pb(1)-I(4)	3.0328(6)	Pb(2)-I(7)	3.0973(5)
Pb(1)-I(2)	3.2633(6)	Pb(2)-I(3)	3.1564(5)
Pb(1)-I(5)	3.4346(5)	Pb(2)-I(5)#1	3.2879(5)
Pb(1)-I(7)#1	3.5068(6)	Pb(2)-I(6)#3	3.6123(6)
Pb(1)-I(7)	3.6036(6)	Pb(2)-I(6)	3.6453(6)
Ag(1)-I(3)#4	2.7366(7)	Ni(1)-N(2)	2.091(5)
Ag(1)-I(5)	2.7787(7)	Ni(1)-N(5)	2.109(5)
Ag(1)-I(6)#1	2.9320(9)	Ni(1)-N(1)	2.125(5)
Ag(1)-I(6)#4	2.9867(9)	Ni(1)-N(4)	2.126(5)
Pb(2)-Ag(1)#2	3.5250(7)	Ni(1)-N(3)	2.128(5)
Pb(2)-Ag(1)#1	3.5552(7)	Ni(1)-N(6)	2.135(5)

Symmetry transformations used to generate equivalent atoms: #1 -*x*, -*y*, -*z*; #2 *x*, *y*-1, *z*; #3 -*x*, -*y*-1, -*z*; #4 *x*, *y*+1, *z*.

Table S2. Selected bond lengths (Å) for compound **2**.

Pb(1)-I(1)	2.9456(7)	Pb(2)-I(2)	3.0620(7)
Pb(1)-I(4)	3.0336(7)	Pb(2)-I(5)	3.0994(6)
Pb(1)-I(2)	3.2653(7)	Pb(2)-I(3)	3.1585(6)
Pb(1)-I(7)	3.4365(6)	Pb(2)-I(7)#1	3.2889(6)
Pb(1)-I(5)#1	3.5084(7)	Pb(2)-I(6)	3.6135(6)
Pb(1)-I(5)	3.6050(7)	Pb(2)-I(6)#3	3.6457(7)
Ag(1)-I(3)#4	2.7393(8)	Co(1)-N(6)	2.098(5)
Ag(1)-I(6)#4	2.9318(9)	Co(1)-N(3)	2.114(5)
Ag(1)-I(6)#1	2.9874(9)	Co(1)-N(1)	2.122(5)
Ag(1)-I(7)	2.7788(8)	Co(1)-N(5)	2.131(5)
Pb(2)-Ag(1)#2	3.5279(8)	Co(1)-N(2)	2.131(5)
Pb(2)-Ag(1)#1	3.5554(7)	Co(1)-N(4)	2.135(5)

Symmetry transformations used to generate equivalent atoms: #1 -*x*, -*y*-1, -*z*-1; #2 *x*, *y*+1, *z*; #3 -*x*, -*y*, -*z*-1, #4 *x*, *y*-1, *z*.

Table S3. Selected bond lengths (Å) for compound **3**.

Pb(1)-I(1)	2.9461(7)	Pb(2)-I(2)	3.0601(7)
Pb(1)-I(4)	3.0337(6)	Pb(2)-I(5)	3.1031(6)
Pb(1)-I(2)	3.2635(7)	Pb(2)-I(3)	3.1659(6)
Pb(1)-I(6)	3.4327(6)	Pb(2)-I(6)#1	3.2876(6)
Pb(1)-I(5)#1	3.5072(7)	Pb(2)-I(7)#3	3.6175(7)
Pb(1)-I(5)	3.5973(7)	Pb(2)-I(7)	3.6519(7)
Ag(1)-I(3)#4	2.7367(9)	Zn(1)-N(2)	2.125(6)
Ag(1)-I(7)#1	2.9347(10)	Zn(1)-N(5)	2.144(6)
Ag(1)-I(7)#4	2.9827(11)	Zn(1)-N(1)	2.149(6)
Ag(1)-I(6)	2.7810(9)	Zn(1)-N(3)	2.163(6)
Pb(2)-Ag(1)#2	3.5199(8)	Zn(1)-N(4)	2.169(6)
Pb(2)-Ag(1)#1	3.5551(8)	Zn(1)-N(6)	2.172(6)

Symmetry transformations used to generate equivalent atoms: #1 -*x*+1, -*y*-1, -*z*; #2 *x*, *y*+1, *z*; #3 -*x*+1, -*y*, -*z*; #4 *x*, *y*-1, *z*.

Table S4. Selected bond lengths (Å) for compound **4**.

Pb(1)-Br(1)	2.7389(10)	Pb(2)-Br(2)	2.8951(10)
Pb(1)-Br(7)	2.8180(9)	Pb(2)-Br(3)	2.9256(9)
Pb(1)-Br(2)	3.0335(10)	Pb(2)-Br(4)	3.0024(9)
Pb(1)-Br(3)#1	3.2836(10)	Pb(2)-Br(6)#1	3.0374(9)
Pb(1)-Br(6)	3.4025(9)	Pb(2)-Br(5)#2	3.2768(10)
Pb(1)-Br(3)	3.4617(10)	Pb(2)-Br(5)	3.3110(10)
Cu(1)-Br(4)#4	2.3383(16)	Co(1)-N(5)	2.104(6)
Cu(1)-Br(5)#4	2.618(2)	Co(1)-N(2)	2.110(6)
Cu(1)-Br(5)#1	2.941(2)	Co(1)-N(4)	2.117(6)
Cu(1)-Br(6)	2.3905(16)	Co(1)-N(1)	2.118(6)
Pb(2)-Cu(1)#3	3.3322(15)	Co(1)-N(3)	2.126(6)
Pb(2)-Cu(1)#1	3.3368(15)	Co(1)-N(6)	2.137(6)

Symmetry transformations used to generate equivalent atoms: #1 -*x*, -*y*-2, -*z*; #2 -*x*, -*y*-1, -*z*; #3 *x*, *y*+1, *z*; #4 *x*, *y*-1, *z*.

Table S5. Selected bond lengths (Å) for compound **5**.

Pb(1)-Br(1)	2.7344(8)	Pb(2)-Br(2)	2.8649(8)
Pb(1)-Br(3)	2.8128(8)	Pb(2)-Br(4)	2.8777(8)
Pb(1)-Br(2)	3.0715(8)	Pb(2)-Br(7)	2.9606(8)
Pb(1)-Br(6)	3.2515(8)	Pb(2)-Br(6)#1	3.1009(8)
Pb(1)-Br(4)#1	3.3482(8)	Pb(2)-Br(5)	3.4315(8)
Pb(1)-Br(4)	3.4665(8)	Pb(2)-Br(5)#2	3.4521(8)
Ag(1)-Br(7)#4	2.5841(9)	Ni(1)-N(2)	2.068(4)
Ag(1)-Br(6)	2.6265(9)	Ni(1)-N(5)	2.072(4)
Ag(1)-Br(5)#1	2.8209(10)	Ni(1)-N(4)	2.075(4)
Ag(1)-Br(5)#4	2.8695(10)	Ni(1)-N(1)	2.078(4)
Pb(2)-Ag(1)#1	3.4756(7)	Ni(1)-N(3)	2.089(4)
Pb(2)-Ag(1)#3	3.4808(7)	Ni(1)-N(6)	2.098(4)

Symmetry transformations used to generate equivalent atoms: #1 -*x*, -*y*-2, -*z*; #2 -*x*, -*y*-1, -*z*; #3 *x*, *y*+1, *z*; #4 *x*, *y*-1, *z*.

Table S6. Selected bond lengths (Å) for compound **6**.

Pb(1)-Br(2)	2.7277(8)	Pb(2)-Br(3)	2.8682(8)
Pb(1)-Br(7)	2.8102(8)	Pb(2)-Br(1)	2.8717(8)

Pb(1)-Br(1)	3.0836(8)	Pb(2)-Br(5)	2.9503(7)
Pb(1)-Br(4)	3.2427(8)	Pb(2)-Br(4)#1	3.1138(8)
Pb(1)-Br(3)#1	3.3787(8)	Pb(2)-Br(6)	3.4361(8)
Pb(1)-Br(3)	3.4923(8)	Pb(2)-Br(6)#2	3.4556(8)
Ag(1)-Br(5)#4	2.5922(9)	Fe(1)-N(2)	1.963(4)
Ag(1)-Br(4)	2.6264(9)	Fe(1)-N(4)	1.964(4)
Ag(1)-Br(6)#1	2.8221(10)	Fe(1)-N(5)	1.967(4)
Ag(1)-Br(6)#4	2.8861(10)	Fe(1)-N(1)	1.974(4)
Pb(2)-Ag(1)#1	3.4674(7)	Fe(1)-N(3)	1.974(4)
Pb(2)-Ag(1)#3	3.4968(8)	Fe(1)-N(6)	1.976(4)

Symmetry transformations used to generate equivalent atoms: #1 -*x*, -*y*-1, -*z*-1; #2 -*x*, -*y*, -*z*-1; #3 *x*, *y*+1, *z*; #4 *x*, *y*-1, *z*.

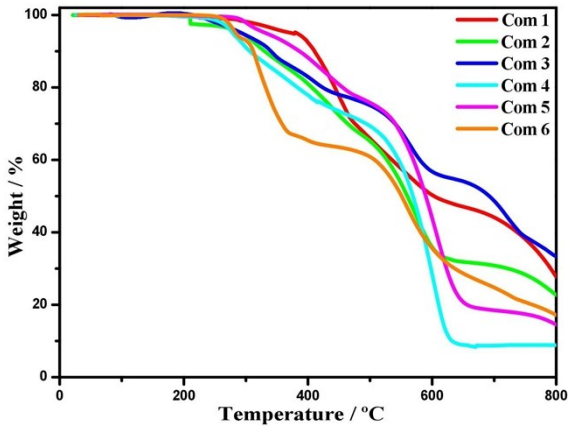

Fig. S1. Thermogravimetric curves for compounds **1**−**6**.

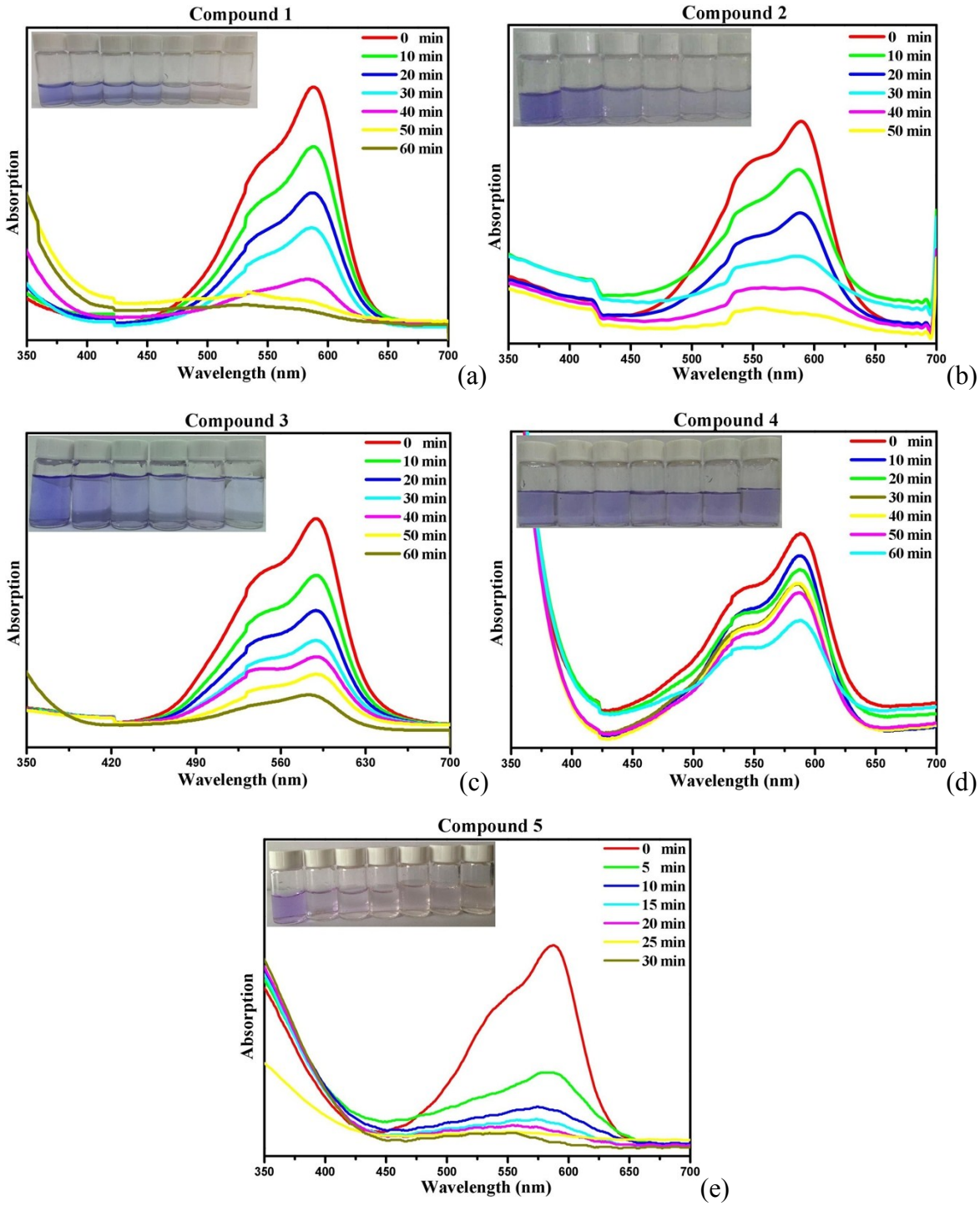

Fig. S2. Absorption spectra of the CV solution in the presence of compounds **1-5** under exposure to visible light (a-e).

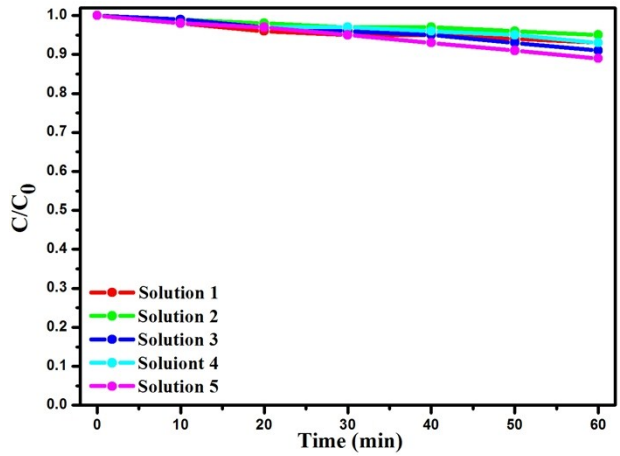

Fig. **S3**. The photodegradation ratios (C_0/C) of CV by solution of samples **1-5** under the visible light irradiation.

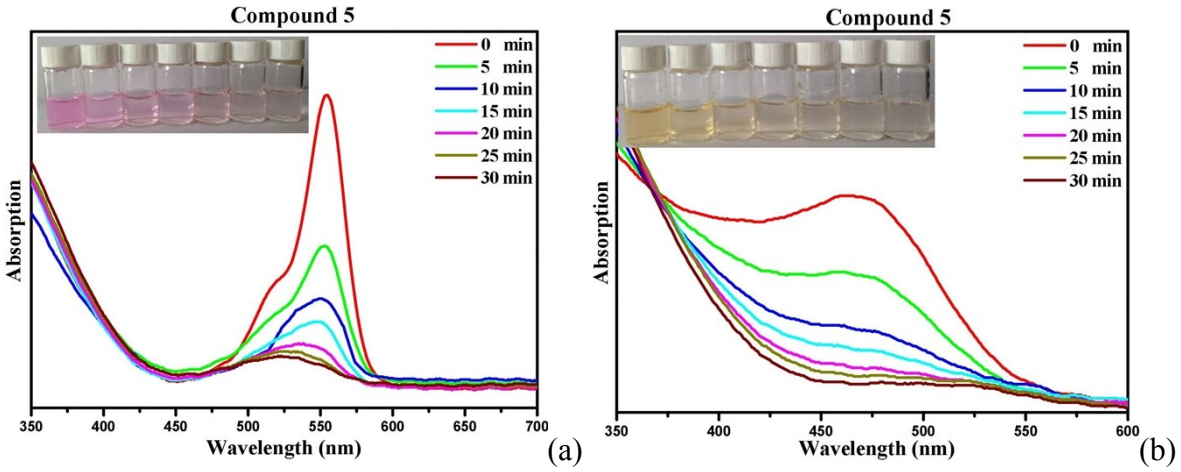

Fig. S4. Absorption spectra of the RhB (a) and MO (b) solution in the presence of compound **5** under exposure to visible light.

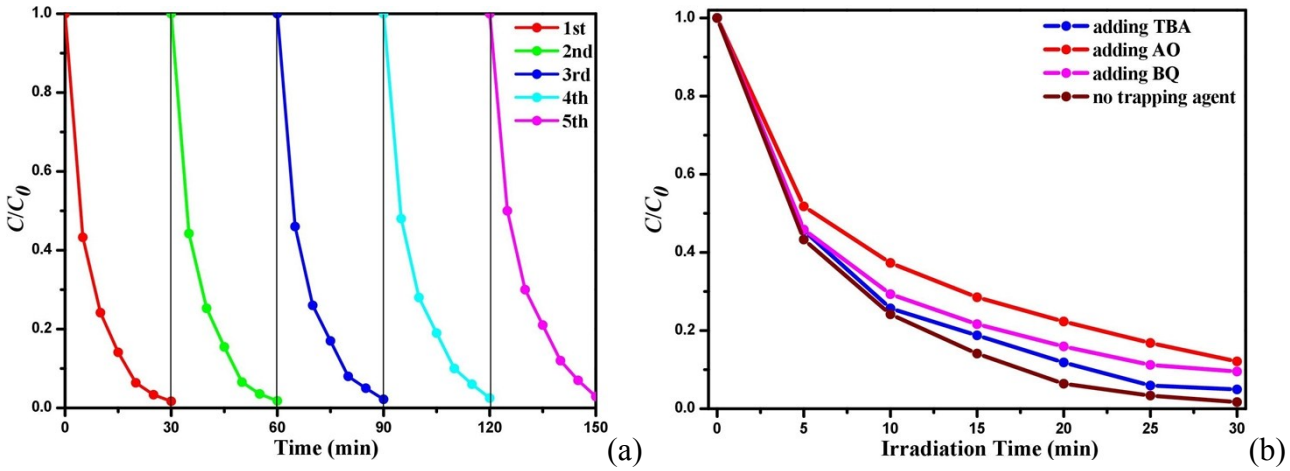

Fig. S5. The recyclability photocatalytic degradation of RhB (a) and radical trapping experiments of RhB over sample **5** under visible light irradiation (b).

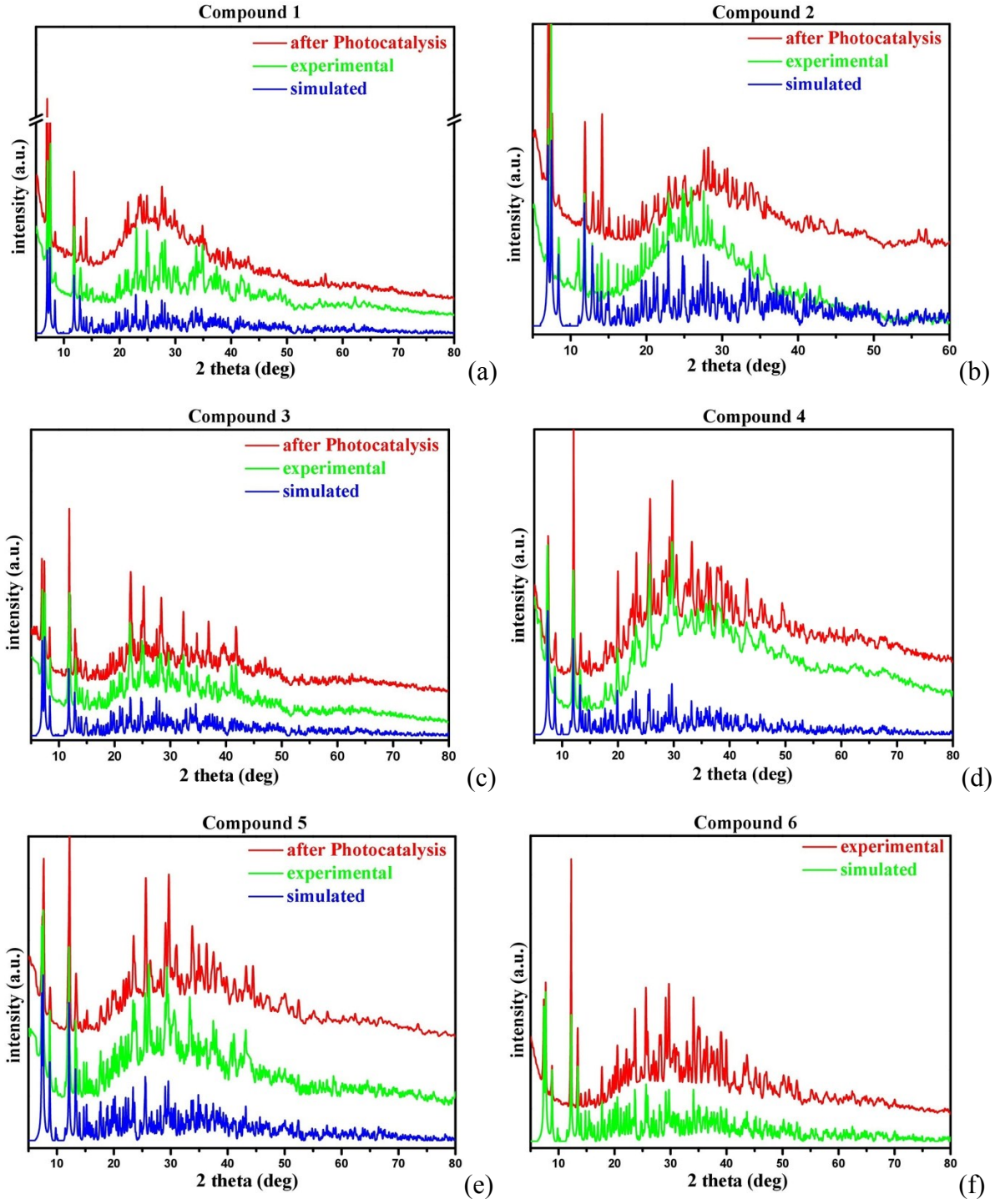

Fig. S6. The experimental and simulated XRD powder patterns for compounds **1-6**.