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Inorganic-organic hybrid compounds based on octamolybdates and multidentate N-donor ligand: syntheses, structures, photoluminescence and photocatalysis

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

Cu(1)-N(1)	2.001(5)	Cu(1)-N(16)#1	2.002(4)
Cu(1)-N(10)	2.024(5)	Cu(1)-N(9)	2.028(5)
Cu(1)-O15	2.548(5)	Cu(1)-O(6W)	2.626(7)
Cu(2)-N(15)	1.976(5)	Cu(2)-N(8)#2	2.003(5)
Cu(2)-N(6)#3	2.010(5)	Cu(2)-N(7)#3	2.026(5)
Cu(2)-O(2W)	2.482(6)	Cu(2)-O(7)#5	2.787(5)
N(1)-Cu(1)-N(16)#1	88.59(19)	N(1)-Cu(1)-N(10)	173.81(17)
N(16)#1-Cu(1)-N(10)	97.42(19)	N(1)-Cu(1)-N(9)	93.3(2)
N(16)#1-Cu(1)-N(9)	174.9(2)	N(10)-Cu(1)-N(9)	80.8(2)
O(15)-Cu(1)-N(10)	94.8(2)	O(15)-Cu(1)-N(9)	97.2(2)
O(15)-Cu(1)-N(1)	83.9(2)	O(15)-Cu(1)-N(16)#3	87.6(2)
O(15)-Cu(1)-O(6W)	173.4(2)	O(6W)-Cu(1)-N(16)#3	93.3(2)
O(6W)-Cu(1)-N(10)	91.6(2)	O(6W)-Cu(1)-N(9)	82.1(2)
O(6W)-Cu(1)-N(1)	89.5(2)	O(2W)-Cu(2)-N(15)	93.5(2)
O(2W)-Cu(2)-N(8)#1	91.2(2)	O(2W)-Cu(2)-N(6)#2	86.8(2)
O(2W)-Cu(2)-N(7)#2	85.8(2)	O(2W)-Cu(2)-O(7)#5	164.9(2)
O(7)#5-Cu(2)-N(15)	90.3(2)	O(7)#5-Cu(2)-N(8)#1	103.6(2)
O(7)#5-Cu(2)-N(6)#2	88.5(2)	O(7)#5-Cu(2)-N(7)#2	79.3(2)
N(15)-Cu(2)-N(8)#2	87.9(2)	N(15)-Cu(2)-N(6)#3	176.37(19)

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N(8)#2-Cu(2)-N(6)#3	95.8(2)	N(15)-Cu(2)-N(7)#3	94.9(2)
N(8)#2-Cu(2)-N(7)#3	176.0(2)	N(6)#3-Cu(2)-N(7)#3	81.5(2)

Symmetry transformations used to generate equivalent atoms: #1 -x - 1, -y, -z; #2 -x, -y, -z + 1; #3 x - 1, y - 1, z; #5 -1 + x, y, z.

Table S2a. Selected bond distances (Å) and angles (°) for **2**.

Cu(1)-N(1)	1.988(3)	Cu(1)-N(6)#1	2.018(3)
Cu(1)-N(8)#2	2.029(4)	Cu(1)-N(7)#1	2.048(4)
Cu(1)-O(1)	2.308(3)	Cu(1)-O(1W)	2.502(3)
N(1)-Cu(1)-N(6)#1	173.61(15)	N(1)-Cu(1)-N(8)#2	88.17(14)
N(6)#1-Cu(1)-N(8)#2	97.69(14)	N(1)-Cu(1)-N(7)#1	93.01(14)
N(6)#1-Cu(1)-N(7)#1	80.87(14)	N(8)#2-Cu(1)-N(7)#1	172.99(14)
N(1)-Cu(1)-O(1)	90.74(13)	N(6)#1-Cu(1)-O(1)	91.31(12)
O(1W)-Cu(1)-N(1)	91.70(13)	O(1W)-Cu(1)-N(7)#1	83.19(12)
O(1W)-Cu(1)-N(8)#2	89.85(12)	O(1W)-Cu(1)-N(6)#1	85.86(13)
O(1W)-Cu(1)-O(1)	175.09(10)	N(8)#2-Cu(1)-O(1)	94.48(13)
N(7)#1-Cu(1)-O(1)	92.41(12)		

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

Table S2b. Hydrogen bonds for **2**.

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1A)···O(12)#6	0.83	2.07	2.829(5)	152.3
O(1W)-H(1B)···O(2W)#6	0.85	2.04	2.800(6)	148.4

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O(2W)-H(2B)···N(2)#3	0.86	2.06	2.886(6)	160.5

Symmetry transformations used to generate equivalent atoms: [#3] -x, -y, -z; [#6] x + 1/2, -y + 1/2, z - 1/2.

Table S3a. Selected bond distances (Å) and angles (°) for **3**.

Co(1)-O(1W)	2.040(3)	Co(1)-O(9)#2	2.073(3)
Co(1)-O(1)	2.110(3)		
O(1W)-Co(1)-O(9)#2	90.11(14)	O(1W)#1-Co(1)-O(9)#2	89.89(14)
O(1W)-Co(1)-O(1)	92.34(14)	O(9)#2-Co(1)-O(1)	92.45(13)
O(1W)#1-Co(1)-O(1)	87.66(15)	O(9)#2-Co(1)-O(1)#1	87.55(13)

Symmetry transformations used to generate equivalent atoms: [#1] -x + 2, -y + 2, -z; [#2] x + 1, y + 1, z.

Table S3b. Hydrogen bonds for **3**.

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1A)···O(10)#5	0.85	1.91	2.753(5)	172.7
O(1W)-H(1B)···O(11)#3	0.85	2.00	2.724(4)	142.1

Symmetry transformations used to generate equivalent atoms: [#3] -x + 1, -y + 1,-z; [#5] -x + 2, -y + 1, -z.

Table S4. Selected bond distances (Å) and angles (°) for **4**.

Zn(1)-O(1W)	2.052(3)	Zn(1)-O(4)	2.086(3)
Zn(1)-O(1)	2.115(3)		
O(1W)-Zn(1)-O(4)#1	89.69(15)	O(1W)-Zn(1)-O(4)	90.31(15)
O(1W)-Zn(1)-O(1)	87.52(13)	O(1W)#1-Zn(1)-O(1)	92.48(13)
O(4)#1-Zn(1)-O(1)	91.58(12)	O(4)-Zn(1)-O(1)	88.42(12)

Symmetry transformations used to generate equivalent atoms: [#1] -x, -y - 1, -z + 1.

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Table S5. Selected bond distances (Å) and angles (°) for **5**.

Ni(1)-O(1W)	2.047(3)	Ni(1)-O(1)	2.051(3)
Ni(1)-N(7)#1	2.087(4)	Ni(1)-N(1)	2.096(4)
Ni(1)-N(8)#2	2.115(4)	Ni(1)-N(2)	2.133(4)
O(1W)-Ni(1)-O(1)	86.08(15)	O(1W)-Ni(1)-N(7)#1	89.84(16)
O(1)-Ni(1)-N(7)#1	174.55(16)	O(1W)-Ni(1)-N(1)	92.61(15)
O(1)-Ni(1)-N(1)	90.05(15)	N(7)#1-Ni(1)-N(1)	86.53(16)
O(1W)-Ni(1)-N(8)#2	91.08(15)	O(1)-Ni(1)-N(8)#2	91.41(15)
N(7)#1-Ni(1)-N(8)#2	92.28(17)	N(1)-Ni(1)-N(8)#2	176.11(16)
O(1W)-Ni(1)-N(2)	170.00(15)	O(1)-Ni(1)-N(2)	89.39(15)
N(7)#1-Ni(1)-N(2)	94.07(16)	N(1)-Ni(1)-N(2)	78.46(16)
N(8)#2-Ni(1)-N(2)	97.95(16)		

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

Table S6a. Selected bond distances (Å) and angles (°) for **6**.

Ag(1)-O(4)#3	2.806(5)	Ag(1)-N(1)	2.189(4)
Ag(1)-O(1)	2.242(4)	Ag(1)-O(4)	2.577(4)
Ag(1)-O(13)#1	2.850(4)		
N(1)-Ag(1)-O(1)	159.14(16)	N(1)-Ag(1)-O(4)	114.90(15)
O(1)-Ag(1)-O(4)	81.12(13)	O(4)#3-Ag(1)-N(1)	107.11(15)
O(4)#3-Ag(1)-O(1)	90.49(13)	O(4)#3-Ag(1)-O(4)	70.31(13)

O(4)#3-Ag(1)-O(13)#1	165.66(12)	O(13)#1-Ag(1)-N(1)	86.90(15)
O(13)#1-Ag(1)-O(1)	75.17(13)	O(13)#1-Ag(1)-O(4)	107.02(13)

Symmetry transformations used to generate equivalent atoms: [#1] -x + 1, -y, -z; [#3] -x, -y + 1, -z.

Table S6b. Hydrogen bonds for **6**.

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N(8)-H(8A)···O(11)#2	0.86	2.26	3.029(5)	148.9

Symmetry transformations used to generate equivalent atoms: [#2] x - 1, y, z - 1.

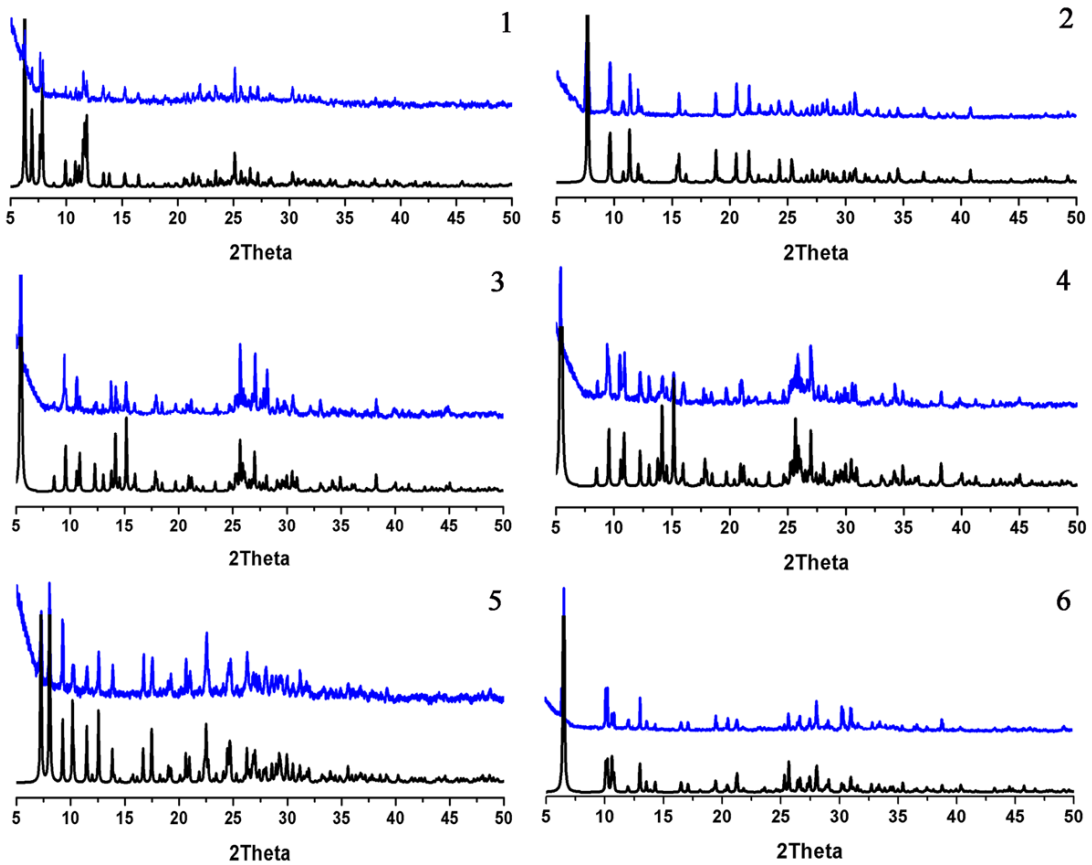

Fig. S1 The simulated (black) and experimental (blue) PXRD patterns for compounds **1**-**6**.

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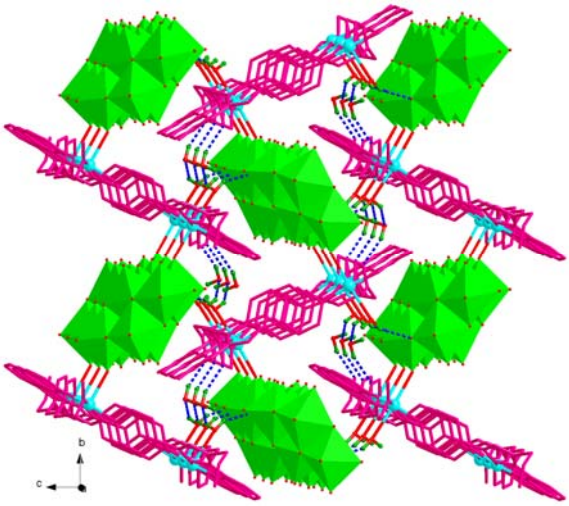

Fig. S2 3D supramolecular framework of **2**.

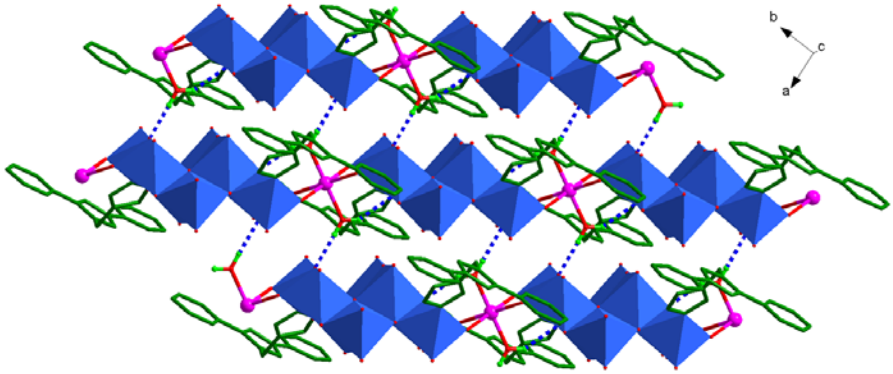

Fig. S3 2D layer formed by the hydrogen bonding interactions in **3**.

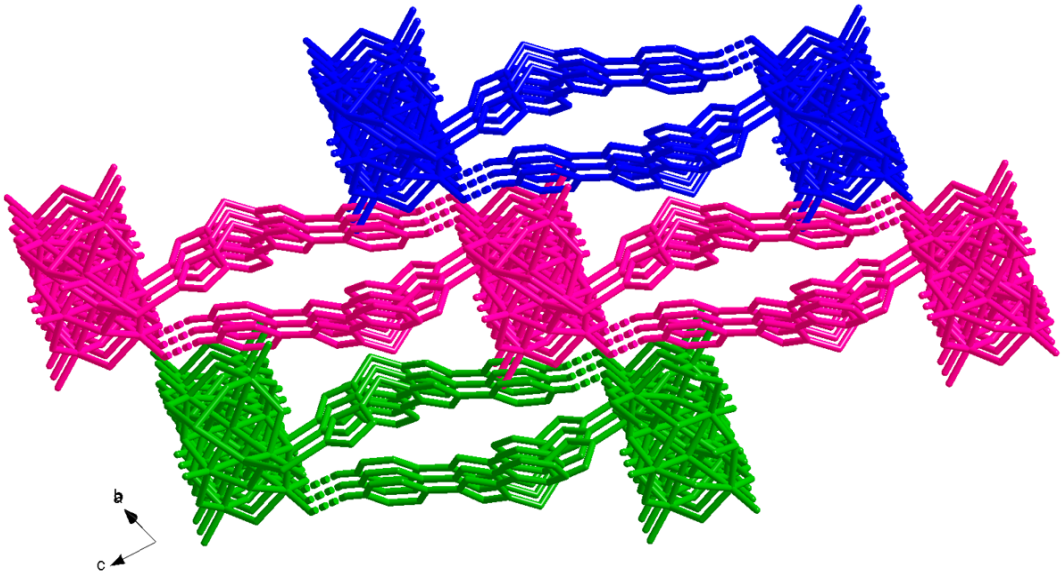

Fig. S4 Interdigitated framework of **6**.

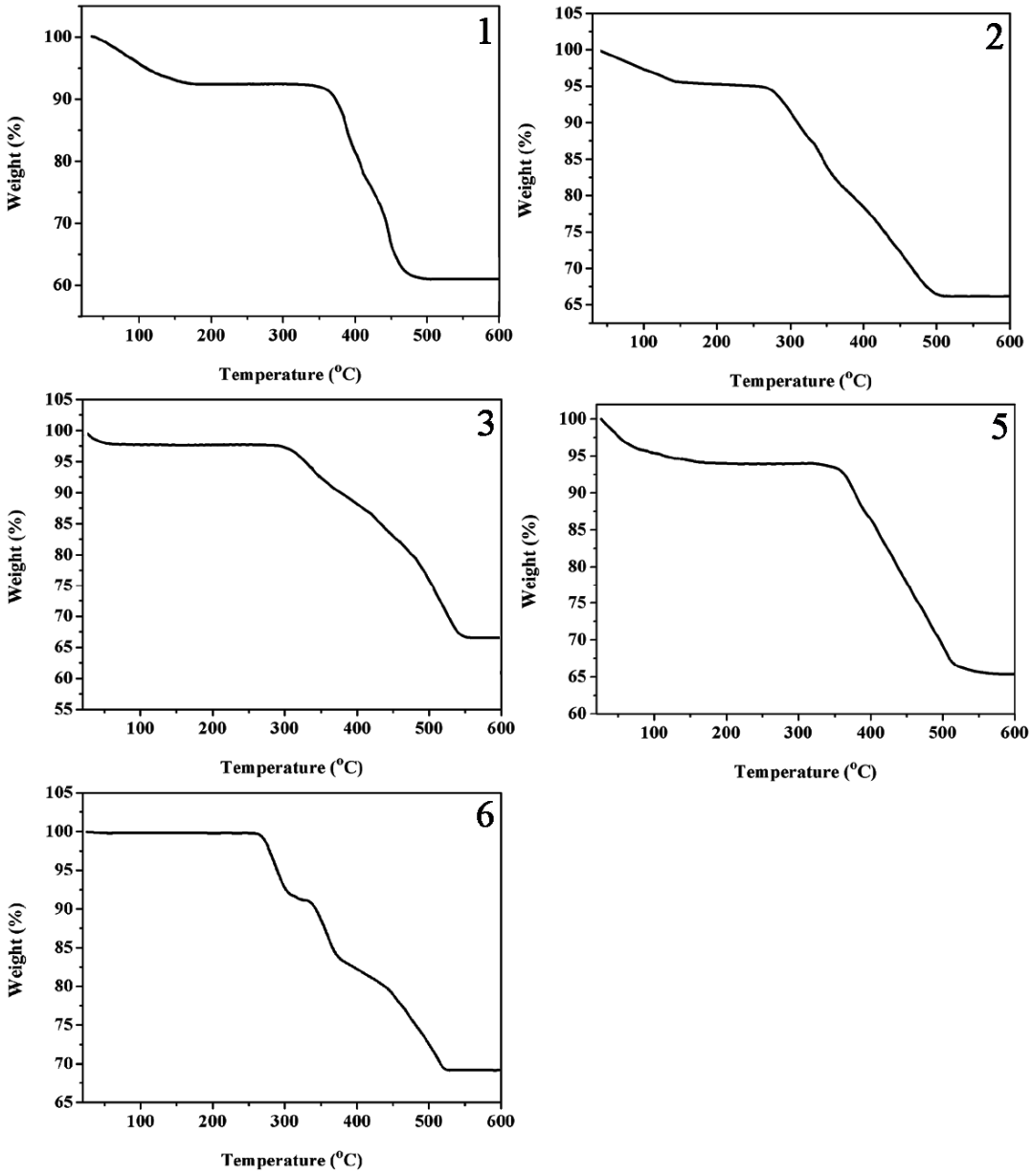

Fig. S5 TGA curves of compounds 1-3, 5 and 6.

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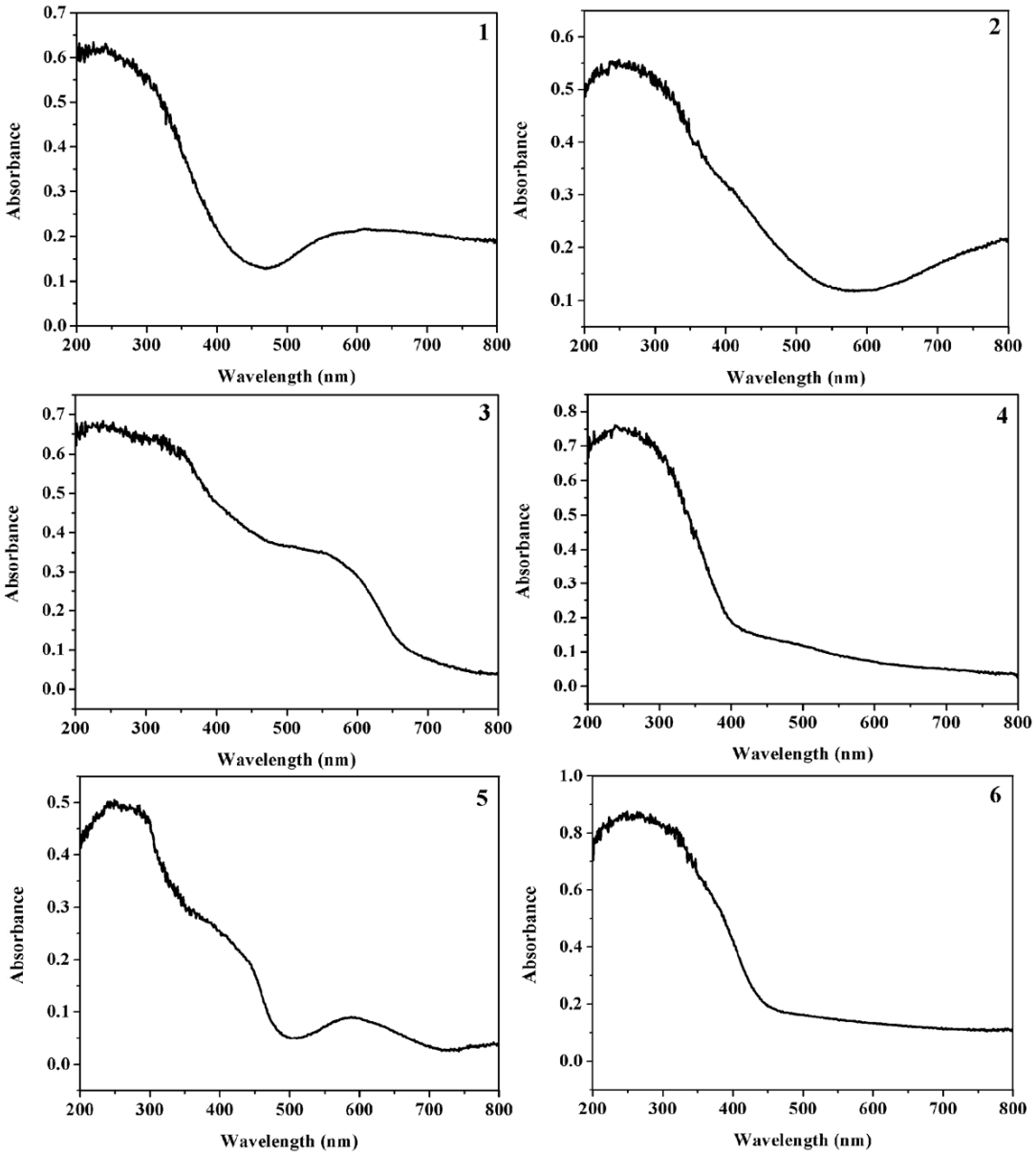

Fig. S6 UV-vis absorption spectra of compounds **1-6.**

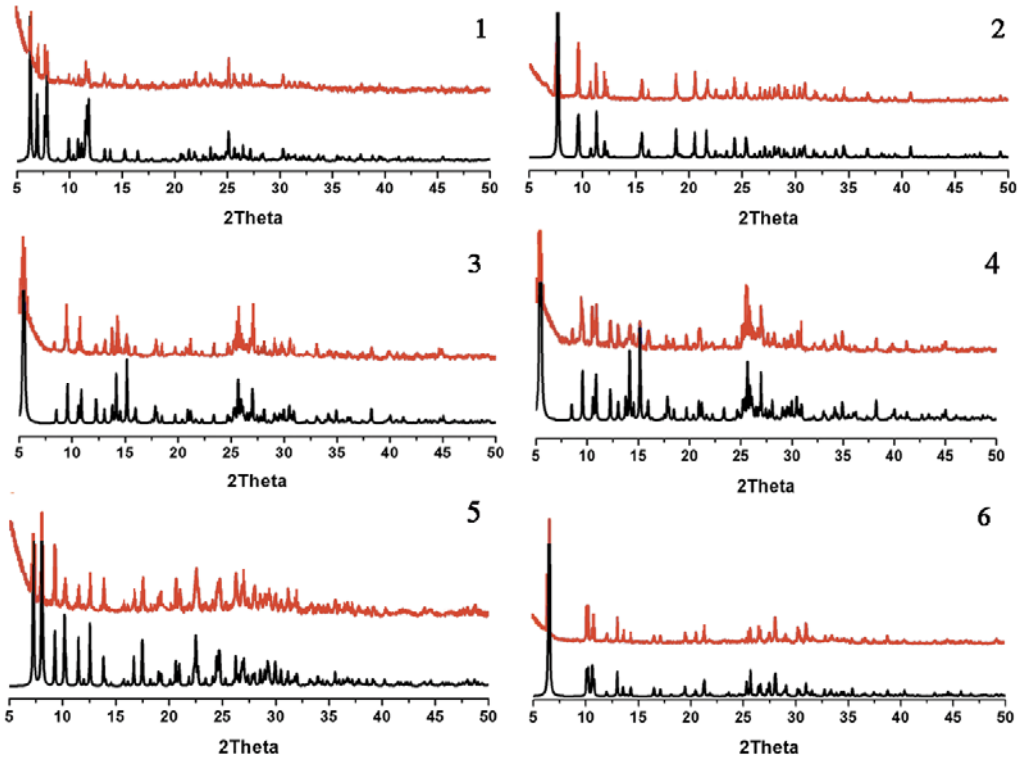

Fig. S7 The simulated (black) PXRD patterns of compounds **1**-**6** and the PXRD patterns of compounds **1**-**6** after photocatalytic processes (red).