Supporting Information

A comparison study of aliphatic and aromatic structure directing agents in influencing the crystal and electronic structures, and property of iodoplumbate hybrids: Water induced structure conversion and visible light photocatalytic property

Guang-Ning Liu,* Jian-Ru Shi, Xiao-Jiang Han, Xiao Zhang, Ke Li, Jie Li, Tao Zhang, Qi-Sheng Liu, Zhen-Wei Zhang, and Cuncheng Li*

[a]*Key Laboratory of Chemical Sensing & Analysis in Universities of Shandong, School of Chemistry and Chemical Engineering, University of Jinan, Jinan, Shandong 250022, P. R. China*

Table S1. Bond Distances (Å) and Angles (°) for **1–6**.

1			
Bond	(Å)	Bond	(Å)
Pb(1)-I(1)	3.1965(3)	N(4)-H(4A)	0.8900
Pb(1)-I(1)#1	3.1965(3)	N(4)-H(4B)	0.8900
Pb(1)-I(2)	3.2132(3)	N(4)-H(4E)	0.8900
Pb(1)-I(2)#1	3.2132(3)	C(1)-C(1)#2	1.483(4)
Pb(1)-I(3)	3.2906(3)	C(1)-H(1D)	0.9700
Pb(1)-I(3)#1	3.2906(3)	C(1)-H(1E)	0.9700
N(1)-C(1)	1.454(4)	C(2)-C(3)	1.498(8)
N(1)-H(1A)	0.8900	C(2)-H(2D)	0.9700
N(1)-H(1B)	0.8900	C(2)-H(2E)	0.9700
N(1)-H(1C)	0.8900	C(3)-H(3C)	0.9700
N(2)-C(2)	1.454(7)	C(3)-H(3D)	0.9700
N(2)-H(2A)	0.8900	C(4)-C(4)#3	1.524(9)
N(2)-H(2B)	0.8900	C(4)-H(4C)	0.9700
N(2)-H(2C)	0.8900	C(4)-H(4D)	0.9700
N(3)-C(3)	1.446(6)	O(1W)-H(1I)	0.8499

N(3)-H(3B)	0.8900	O(1W)-H(1F)	0.820(5)
N(3)-H(3E)	0.8900	O(1W)-H(1G)	0.820(4)
N(4)-C(4)	1.478(6)	O(1W)-H(1H)	0.819(5)

Angle	(°)	Angle	(°)
I(1)-Pb(1)-I(1)#1	103.093(12)	C(4)-N(4)-H(4A)	109.5
I(1)-Pb(1)-I(2)	87.001(8)	C(4)-N(4)-H(4B)	109.5
I(1)#1-Pb(1)-I(2)	91.629(8)	C(4)-N(4)-H(4E)	109.5
I(1)-Pb(1)-I(2)#1	91.629(8)	N(1)-C(1)-C(1)#2	113.0(4)
I(1)#1-Pb(1)-I(2)#1	87.001(8)	N(1)-C(1)-H(1D)	109.0
I(2)-Pb(1)-I(2)#1	177.798(13)	C(1)#2-C(1)-H(1D)	109.0
I(1)-Pb(1)-I(3)	166.607(8)	N(1)-C(1)-H(1E)	109.0
I(1)#1-Pb(1)-I(3)	87.964(8)	C(1)#2-C(1)-H(1E)	109.0
I(2)-Pb(1)-I(3)	85.129(8)	N(2)-C(2)-C(3)	113.9(4)
I(2)#1-Pb(1)-I(3)	96.539(8)	N(2)-C(2)-H(2D)	108.8
I(1)-Pb(1)-I(3)#1	87.964(8)	C(3)-C(2)-H(2D)	108.8
I(1)#1-Pb(1)-I(3)#1	166.607(8)	N(2)-C(2)-H(2E)	108.8
I(2)-Pb(1)-I(3)#1	96.539(8)	C(3)-C(2)-H(2E)	108.8
I(2)#1-Pb(1)-I(3)#1	85.129(8)	N(3)-C(3)-C(2)	116.0(5)
I(3)-Pb(1)-I(3)#1	82.196(11)	N(3)-C(3)-H(3C)	108.3
C(1)-N(1)-H(1A)	109.5	C(2)-C(3)-H(3C)	108.3
C(1)-N(1)-H(1B)	109.5	N(3)-C(3)-H(3D)	108.3
C(1)-N(1)-H(1C)	109.5	C(2)-C(3)-H(3D)	108.3
C(2)-N(2)-H(2A)	109.5	N(4)-C(4)-C(4)#3	111.2(5)
C(2)-N(2)-H(2B)	109.5	N(4)-C(4)-H(4C)	109.4
C(2)-N(2)-H(2C)	109.5	C(4)#3-C(4)-H(4C)	109.4
C(3)-N(3)-H(3B)	109.1	N(4)-C(4)-H(4D)	109.4
C(3)-N(3)-H(3E)	109.4	C(4)#3-C(4)-H(4D)	109.4

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

-z+1; #3 -x+1, -y+1, -z+1.

2			
Bond	(Å)	Bond	(Å)
Pb(1)-I(2)#1	3.1711(4)	Pb(2)-N(1)	2.360(3)
Pb(1)-I(2)	3.1711(4)	Pb(2)-I(3)#5	3.2079(2)
Pb(1)-I(1)#1	3.2202(3)	Pb(2)-I(3)	3.2079(2)
Pb(1)-I(1)	3.2202(3)	I(3)-Pb(2)#13	3.2079(2)
Pb(1)-I(1)#2	3.2202(3)	N(1)-C(1)	1.486(5)
Pb(1)-I(1)#3	3.2202(3)	C(1)-C(1)#4	1.355(8)
Pb(2)-N(1)#4	2.360(3)		
Angle	(°)	Angle	(°)
I(2)#1-Pb(1)-I(2)	180.0	I(2)-Pb(1)-I(1)#3	87.197(7)
I(2)#1-Pb(1)-I(1)#1	87.197(7)	I(1)#1-Pb(1)-I(1)#3	93.471(10)
I(2)-Pb(1)-I(1)#1	92.803(7)	I(1)-Pb(1)-I(1)#3	86.529(10)
I(2)#1-Pb(1)-I(1)	92.803(7)	I(1)#2-Pb(1)-I(1)#3	180.0
I(2)-Pb(1)-I(1)	87.197(7)	N(1)#4-Pb(2)-N(1)	70.71(15)
I(1)#1-Pb(1)-I(1)	180.0	N(1)#4-Pb(2)-I(3)#5	82.24(9)
I(2)#1-Pb(1)-I(1)#2	87.197(7)	N(1)-Pb(2)-I(3)#5	85.07(9)
I(2)-Pb(1)-I(1)#2	92.803(7)	N(1)#4-Pb(2)-I(3)	85.07(9)
I(1)#1-Pb(1)-I(1)#2	86.529(10)	N(1)-Pb(2)-I(3)	82.24(9)
I(1)-Pb(1)-I(1)#2	93.471(10)	I(3)#5-Pb(2)-I(3)	164.435(7)
I(2)#1-Pb(1)-I(1)#3	92.803(7)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y+1, -z+2; #2 x, -y+1, -z+2; #3 -x+1, y, z; #4 -x+1/2, y+0, -z+1/2; #5 -x+1/2, -y+1, z-1/2; #6 -x+1, -y+3/2, z-1/2; #7 x, -y+1, -z+1; #8 -x+1, -y+1, -z+1; #9 -x+1, y+1/2, -z+3/2; #10 x, y+1/2, -z+3/2; #11 x, y-1/2, -z+3/2; #12 -x+1, -y+3/2, z+1/2.

3			
Bond	(Å)	Bond	(Å)
Pb(1)-I(2)	3.0896(3)	N(5)-H(11D)	0.8900
Pb(1)-I(4)	3.1550(3)	N(5)-H(11E)	0.8900
Pb(1)-I(5)	3.2331(3)	C(1)-C(2)	1.496(5)
Pb(1)-I(3)	3.2537(3)	C(1)-H(1A)	0.9700
Pb(1)-I(1)#1	3.2904(3)	C(1)-H(1B)	0.9700
Pb(1)-I(1)	3.3180(2)	C(2)-H(2A)	0.9700
I(1)-Pb(1)#2	3.2904(3)	C(2)-H(2B)	0.9700
N(1)-C(1)	1.489(5)	C(3)-C(4)	1.502(5)
N(1)-H(12A)	0.8900	C(3)-H(3A)	0.9700
N(1)-H(12B)	0.8900	C(3)-H(3B)	0.9700
N(1)-H(12C)	0.8900	C(4)-H(4A)	0.9700
N(2)-C(3)	1.462(5)	C(4)-H(4B)	0.9700
N(2)-C(2)	1.466(4)	C(5)-C(6)	1.507(5)
N(2)-H(2C)	0.8600	C(5)-H(5A)	0.9700
N(3)-C(5)	1.480(4)	C(5)-H(5B)	0.9700
N(3)-C(4)	1.489(4)	C(6)-H(6A)	0.9700
N(3)-H(11A)	0.9000	C(6)-H(6B)	0.9700
N(3)-H(11B)	0.9000	C(7)-C(8)	1.502(5)
N(4)-C(6)	1.449(4)	C(7)-H(7A)	0.9700
N(4)-C(7)	1.464(4)	C(7)-H(7B)	0.9700
N(4)-H(4C)	0.8600	C(8)-H(8A)	0.9700
N(5)-C(8)	1.490(5)	C(8)-H(8B)	0.9700
N(5)-H(11C)	0.8900		
Angle	(°)	Angle	(°)
I(2)-Pb(1)-I(4)	96.321(7)	C(2)-C(1)-H(1B)	109.7
I(2)-Pb(1)-I(5)	90.919(8)	H(1A)-C(1)-H(1B)	108.2

I(4)-Pb(1)-I(5)	94.828(7)	N(2)-C(2)-C(1)	110.4(3)
I(2)-Pb(1)-I(3)	94.730(8)	N(2)-C(2)-H(2A)	109.6
I(4)-Pb(1)-I(3)	88.651(7)	C(1)-C(2)-H(2A)	109.6
I(5)-Pb(1)-I(3)	173.009(7)	N(2)-C(2)-H(2B)	109.6
I(2)-Pb(1)-I(1)#1	88.251(7)	C(1)-C(2)-H(2B)	109.6
I(4)-Pb(1)-I(1)#1	174.914(7)	H(2A)-C(2)-H(2B)	108.1
I(5)-Pb(1)-I(1)#1	82.841(7)	N(2)-C(3)-C(4)	109.4(3)
I(3)-Pb(1)-I(1)#1	93.200(7)	N(2)-C(3)-H(3A)	109.8
I(2)-Pb(1)-I(1)	172.755(7)	C(4)-C(3)-H(3A)	109.8
I(4)-Pb(1)-I(1)	90.806(7)	N(2)-C(3)-H(3B)	109.8
I(5)-Pb(1)-I(1)	89.772(7)	C(4)-C(3)-H(3B)	109.8
I(3)-Pb(1)-I(1)	84.109(7)	H(3A)-C(3)-H(3B)	108.2
I(1)#1-Pb(1)-I(1)	84.679(4)	N(3)-C(4)-C(3)	112.0(3)
Pb(1)#2-I(1)-Pb(1)	165.933(8)	N(3)-C(4)-H(4A)	109.2
C(1)-N(1)-H(12A)	109.5	C(3)-C(4)-H(4A)	109.2
C(1)-N(1)-H(12B)	109.5	N(3)-C(4)-H(4B)	109.2
H(12A)-N(1)-H(12B)	109.5	C(3)-C(4)-H(4B)	109.2
C(1)-N(1)-H(12C)	109.5	H(4A)-C(4)-H(4B)	107.9
H(12A)-N(1)-H(12C)	109.5	N(3)-C(5)-C(6)	111.2(3)
H(12B)-N(1)-H(12C)	109.5	N(3)-C(5)-H(5A)	109.4
C(3)-N(2)-C(2)	113.3(3)	C(6)-C(5)-H(5A)	109.4
C(3)-N(2)-H(2C)	123.4	N(3)-C(5)-H(5B)	109.4
C(2)-N(2)-H(2C)	123.4	C(6)-C(5)-H(5B)	109.4
C(5)-N(3)-C(4)	113.2(3)	H(5A)-C(5)-H(5B)	108.0
C(5)-N(3)-H(11A)	108.9	N(4)-C(6)-C(5)	111.6(3)
C(4)-N(3)-H(11A)	108.9	N(4)-C(6)-H(6A)	109.3
C(5)-N(3)-H(11B)	108.9	C(5)-C(6)-H(6A)	109.3
C(4)-N(3)-H(11B)	108.9	N(4)-C(6)-H(6B)	109.3
H(11A)-N(3)-H(11B)	107.7	C(5)-C(6)-H(6B)	109.3

C(6)-N(4)-C(7)	112.2(3)	H(6A)-C(6)-H(6B)	108.0
C(6)-N(4)-H(4C)	123.9	N(4)-C(7)-C(8)	111.7(3)
C(7)-N(4)-H(4C)	123.9	N(4)-C(7)-H(7A)	109.3
C(8)-N(5)-H(11C)	109.5	C(8)-C(7)-H(7A)	109.3
C(8)-N(5)-H(11D)	109.5	N(4)-C(7)-H(7B)	109.3
H(11C)-N(5)-H(11D)	109.5	C(8)-C(7)-H(7B)	109.3
C(8)-N(5)-H(11E)	109.5	H(7A)-C(7)-H(7B)	107.9
H(11C)-N(5)-H(11E)	109.5	N(5)-C(8)-C(7)	109.6(3)
H(11D)-N(5)-H(11E)	109.5	N(5)-C(8)-H(8A)	109.8
N(1)-C(1)-C(2)	109.9(3)	C(7)-C(8)-H(8A)	109.8
N(1)-C(1)-H(1A)	109.7	N(5)-C(8)-H(8B)	109.8
C(2)-C(1)-H(1A)	109.7	C(7)-C(8)-H(8B)	109.8
N(1)-C(1)-H(1B)	109.7	H(8A)-C(8)-H(8B)	108.2

Symmetry transformations used to generate equivalent atoms:

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

4			
Bond	(Å)	Bond	(Å)
Pb(1)-I(1)	3.1397(3)	N(3)-H(12B)	0.9000
Pb(1)-I(3)	3.1974(3)	C(1)-C(2)	1.497(6)
Pb(1)-I(4)#1	3.2321(3)	C(1)-H(1A)	0.9700
Pb(1)-I(2)	3.2509(3)	C(1)-H(1B)	0.9700
Pb(1)-I(4)	3.2529(3)	C(2)-H(2A)	0.9700
Pb(1)-I(2)#2	3.2831(3)	C(2)-H(2B)	0.9700
N(1)-C(6)	1.487(6)	C(3)-C(4)	1.504(5)
N(1)-H(11A)	0.8900	C(3)-H(3A)	0.9700
N(1)-H(11B)	0.8900	C(3)-H(3B)	0.9700
N(1)-H(11C)	0.8900	C(4)-H(4A)	0.9700
N(2)-C(5)	1.454(5)	C(4)-H(4B)	0.9700

N(2)-C(4)	1.469(5)	C(5)-C(6)	1.490(6)
N(2)-C(2)	1.470(5)	C(5)-H(5A)	0.9700
N(3)-C(1)	1.489(5)	C(5)-H(5B)	0.9700
N(3)-C(3)	1.504(5)	C(6)-H(6A)	0.9700
N(3)-H(12A)	0.9000	C(6)-H(6B)	0.9700
Angle	(°)	Angle	(°)
I(1)-Pb(1)-I(3)	175.490(9)	C(2)-C(1)-H(1A)	109.2
I(1)-Pb(1)-I(4)#1	93.756(8)	N(3)-C(1)-H(1B)	109.2
I(3)-Pb(1)-I(4)#1	86.037(7)	C(2)-C(1)-H(1B)	109.2
I(1)-Pb(1)-I(2)	90.817(8)	H(1A)-C(1)-H(1B)	107.9
I(3)-Pb(1)-I(2)	93.673(8)	N(2)-C(2)-C(1)	109.2(3)
I(4)#1-Pb(1)-I(2)	87.507(8)	N(2)-C(2)-H(2A)	109.8
I(1)-Pb(1)-I(4)	91.663(8)	C(1)-C(2)-H(2A)	109.8
I(3)-Pb(1)-I(4)	83.829(7)	N(2)-C(2)-H(2B)	109.8
I(4)#1-Pb(1)-I(4)	88.715(5)	C(1)-C(2)-H(2B)	109.8
I(2)-Pb(1)-I(4)	175.609(8)	H(2A)-C(2)-H(2B)	108.3
I(1)-Pb(1)-I(2)#2	94.880(8)	C(4)-C(3)-N(3)	111.0(3)
I(3)-Pb(1)-I(2)#2	85.646(8)	C(4)-C(3)-H(3A)	109.4
I(4)#1-Pb(1)-I(2)#2	170.592(8)	N(3)-C(3)-H(3A)	109.4
I(2)-Pb(1)-I(2)#2	88.644(5)	C(4)-C(3)-H(3B)	109.4
I(4)-Pb(1)-I(2)#2	94.753(8)	N(3)-C(3)-H(3B)	109.4
Pb(1)-I(2)-Pb(1)#3	153.871(10)	H(3A)-C(3)-H(3B)	108.0
Pb(1)#4-I(4)-Pb(1)	163.264(10)	N(2)-C(4)-C(3)	109.6(3)
C(6)-N(1)-H(11A)	109.5	N(2)-C(4)-H(4A)	109.8
C(6)-N(1)-H(11B)	109.5	C(3)-C(4)-H(4A)	109.8
H(11A)-N(1)-H(11B)	109.5	N(2)-C(4)-H(4B)	109.8
C(6)-N(1)-H(11C)	109.5	C(3)-C(4)-H(4B)	109.8
H(11A)-N(1)-H(11C)	109.5	H(4A)-C(4)-H(4B)	108.2

H(11B)-N(1)-H(11C)	109.5	N(2)-C(5)-C(6)	112.8(3)
C(5)-N(2)-C(4)	111.5(3)	N(2)-C(5)-H(5A)	109.0
C(5)-N(2)-C(2)	110.8(3)	C(6)-C(5)-H(5A)	109.0
C(4)-N(2)-C(2)	108.4(3)	N(2)-C(5)-H(5B)	109.0
C(1)-N(3)-C(3)	109.7(3)	C(6)-C(5)-H(5B)	109.0
C(1)-N(3)-H(12A)	109.7	H(5A)-C(5)-H(5B)	107.8
C(3)-N(3)-H(12A)	109.7	N(1)-C(6)-C(5)	108.1(3)
C(1)-N(3)-H(12B)	109.7	N(1)-C(6)-H(6A)	110.1
C(3)-N(3)-H(12B)	109.7	C(5)-C(6)-H(6A)	110.1
H(12A)-N(3)-H(12B)	108.2	N(1)-C(6)-H(6B)	110.1
N(3)-C(1)-C(2)	112.2(3)	C(5)-C(6)-H(6B)	110.1
N(3)-C(1)-H(1A)	109.2	H(6A)-C(6)-H(6B)	108.4

Symmetry transformations used to generate equivalent atoms:

#1: -x, y+1/2, -z+1/2; #2: -x+1/2, y-1/2, z; #3: -x+1/2, y+1/2, z; #4: -x, y-1/2, -z+1/2.

5			
Bond	(Å)	Bond	(Å)
Pb(1)-I(1)	3.1575(3)	N(1)-C(1)	1.353(6)
Pb(1)-I(4)	3.1704(3)	N(1)-C(21)	1.479(5)
Pb(1)-I(5)	3.2298(3)	N(2)-C(10)	1.342(5)
Pb(1)-I(2)	3.2313(3)	N(2)-C(6)	1.363(5)
Pb(1)-I(3)	3.3340(3)	N(2)-C(11)	1.494(5)
Pb(1)-I(6)	3.4005(4)	C(1)-C(2)	1.348(7)
Pb(2)-I(6)#1	3.1197(4)	C(2)-C(3)	1.377(7)
Pb(2)-I(3)	3.1613(3)	C(3)-C(4)	1.371(6)
Pb(2)-I(2)	3.2133(3)	C(4)-C(5)	1.373(6)
Pb(2)-I(5)#1	3.2391(3)	C(5)-C(6)	1.501(5)
Pb(2)-I(4)#1	3.2395(3)	C(6)-C(7)	1.367(5)
Pb(2)-I(1)	3.3103(3)	C(7)-C(8)	1.371(6)

I(4)-Pb(2)#2	3.2395(3)	C(8)-C(9)	1.353(6)
I(5)-Pb(2)#2	3.2391(3)	C(9)-C(10)	1.370(6)
I(6)-Pb(2)#2	3.1197(4)	C(11)-C(12)	1.425(7)
N(1)-C(5)	1.349(5)	C(21)-C(22)	1.470(6)
Angle	(°)	Angle	(°)
I(1)-Pb(1)-I(4)	86.882(9)	I(5)#1-Pb(2)-I(1)	89.882(8)
I(1)-Pb(1)-I(5)	101.407(9)	I(4)#1-Pb(2)-I(1)	97.883(9)
I(4)-Pb(1)-I(5)	86.473(8)	Pb(1)-I(1)-Pb(2)	74.472(8)
I(1)-Pb(1)-I(2)	86.341(9)	Pb(2)-I(2)-Pb(1)	74.827(8)
I(4)-Pb(1)-I(2)	101.854(8)	Pb(2)-I(3)-Pb(1)	74.091(7)
I(5)-Pb(1)-I(2)	169.012(9)	Pb(1)-I(4)-Pb(2)#2	76.791(7)
I(1)-Pb(1)-I(3)	86.267(9)	Pb(1)-I(5)-Pb(2)#2	75.972(7)
I(4)-Pb(1)-I(3)	167.509(9)	Pb(2)#2-I(6)-Pb(1)	75.132(8)
I(5)-Pb(1)-I(3)	84.662(8)	C(5)-N(1)-C(1)	119.8(4)
I(2)-Pb(1)-I(3)	88.119(8)	C(5)-N(1)-C(21)	122.8(4)
I(1)-Pb(1)-I(6)	168.245(9)	C(1)-N(1)-C(21)	117.4(4)
I(4)-Pb(1)-I(6)	83.565(8)	C(10)-N(2)-C(6)	120.7(3)
I(5)-Pb(1)-I(6)	84.861(8)	C(10)-N(2)-C(11)	118.8(3)
I(2)-Pb(1)-I(6)	88.927(9)	C(6)-N(2)-C(11)	120.4(3)
I(3)-Pb(1)-I(6)	104.341(9)	C(2)-C(1)-N(1)	122.2(4)
I(6)#1-Pb(2)-I(3)	94.742(9)	C(1)-C(2)-C(3)	118.7(4)
I(6)#1-Pb(2)-I(2)	90.924(9)	C(4)-C(3)-C(2)	119.3(5)
I(3)-Pb(2)-I(2)	91.496(9)	C(3)-C(4)-C(5)	120.5(4)
I(6)#1-Pb(2)-I(5)#1	89.444(9)	N(1)-C(5)-C(4)	119.4(4)
I(3)-Pb(2)-I(5)#1	171.310(9)	N(1)-C(5)-C(6)	120.0(3)
I(2)-Pb(2)-I(5)#1	96.055(8)	C(4)-C(5)-C(6)	120.5(4)
I(6)#1-Pb(2)-I(4)#1	87.085(9)	N(2)-C(6)-C(7)	119.2(3)
I(3)-Pb(2)-I(4)#1	87.425(8)	N(2)-C(6)-C(5)	120.2(3)

I(2)-Pb(2)-I(4)#1	177.649(9)	C(7)-C(6)-C(5)	120.6(3)
I(5)#1-Pb(2)-I(4)#1	85.182(8)	C(6)-C(7)-C(8)	120.2(4)
I(6)#1-Pb(2)-I(1)	174.913(9)	C(9)-C(8)-C(7)	119.7(4)
I(3)-Pb(2)-I(1)	86.609(9)	C(8)-C(9)-C(10)	119.9(4)
I(2)-Pb(2)-I(1)	84.133(9)	N(2)-C(10)-C(9)	120.3(4)
I(1)-Pb(1)-I(4)	86.882(9)	C(12)-C(11)-N(2)	116.7(4)

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

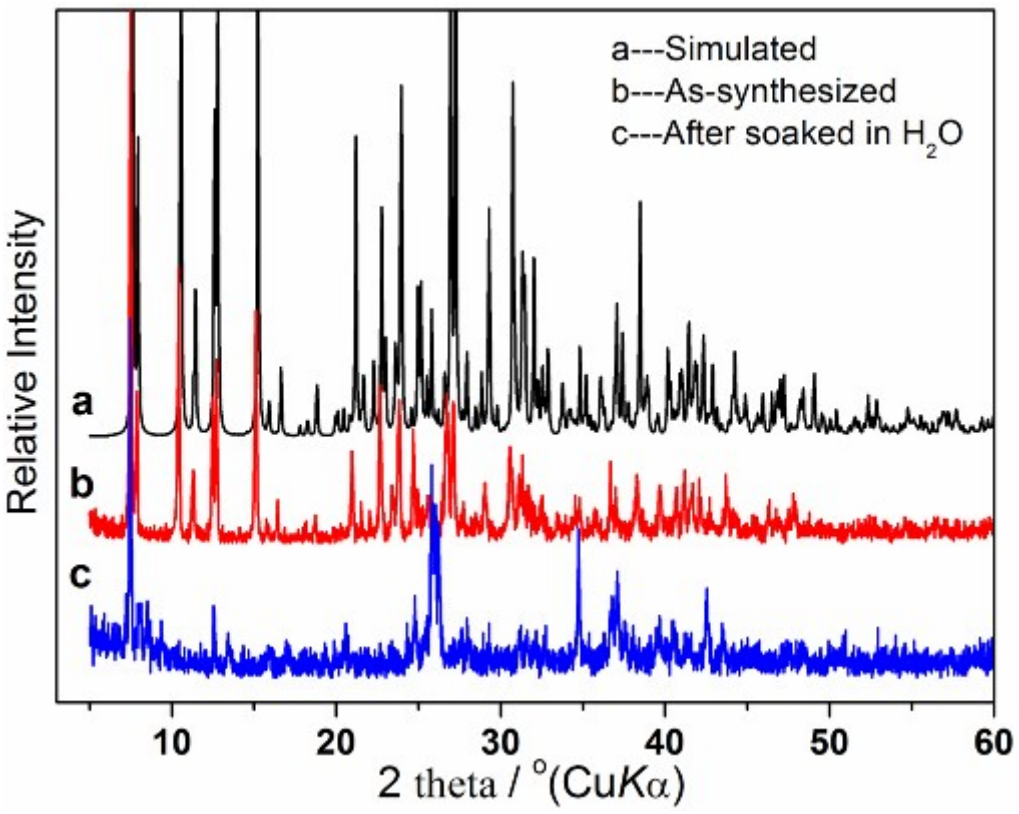
6

Bond	(Å)	Bond	(Å)
Pb(1)-I(2)#1	3.2118(3)	N(1)-C(4)	1.332(5)
Pb(1)-I(1)#2	3.2136(3)	N(1)-C(7)	1.491(6)
Pb(1)-I(1)	3.2205(3)	C(1)-C(1)#3	1.319(7)
Pb(1)-I(3)#2	3.2292(3)	C(1)-C(2)	1.458(5)
Pb(1)-I(3)	3.2357(3)	C(2)-C(3)	1.381(6)
Pb(1)-I(2)	3.2670(3)	C(2)-C(5)	1.391(5)
I(1)-Pb(1)#1	3.2136(3)	C(3)-C(4)	1.386(6)
I(2)-Pb(1)#2	3.2118(3)	C(5)-C(6)	1.372(6)
I(3)-Pb(1)#1	3.2292(3)	C(7)-C(8)	1.459(6)
N(1)-C(6)	1.312(6)		

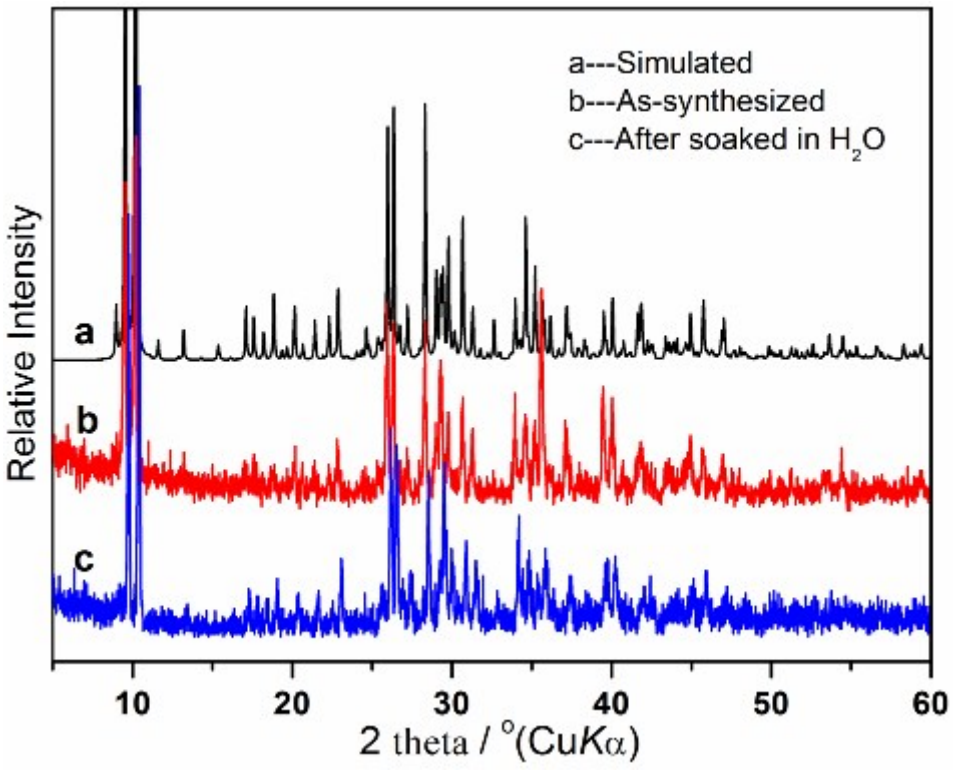
Angle	(°)	Angle	(°)
I(2)#1-Pb(1)-I(1)#2	90.865(7)	Pb(1)#1-I(1)-Pb(1)	76.645(7)
I(2)#1-Pb(1)-I(1)	87.275(8)	Pb(1)#2-I(2)-Pb(1)	76.015(6)
I(1)#2-Pb(1)-I(1)	100.529(10)	Pb(1)#1-I(3)-Pb(1)	76.214(7)
I(2)#1-Pb(1)-I(3)#2	100.513(8)	C(6)-N(1)-C(4)	119.3(4)
I(1)#2-Pb(1)-I(3)#2	86.137(8)	C(6)-N(1)-C(7)	118.6(3)
I(1)-Pb(1)-I(3)#2	169.738(8)	C(4)-N(1)-C(7)	122.0(4)

I(2)#1-Pb(1)-I(3)	85.035(7)	C(1)#3-C(1)-C(2)	125.9(4)
I(1)#2-Pb(1)-I(3)	172.210(8)	C(3)-C(2)-C(5)	116.3(4)
I(1)-Pb(1)-I(3)	85.915(8)	C(3)-C(2)-C(1)	120.5(3)
I(3)#2-Pb(1)-I(3)	88.100(9)	C(5)-C(2)-C(1)	123.2(4)
I(2)#1-Pb(1)-I(2)	174.383(11)	C(2)-C(3)-C(4)	120.9(3)
I(1)#2-Pb(1)-I(2)	86.461(7)	N(1)-C(4)-C(3)	120.8(4)
I(1)-Pb(1)-I(2)	88.357(8)	C(6)-C(5)-C(2)	119.7(4)
I(3)#2-Pb(1)-I(2)	84.248(8)	N(1)-C(6)-C(5)	122.9(4)
I(3)-Pb(1)-I(2)	98.178(7)	C(8)-C(7)-N(1)	111.4(4)

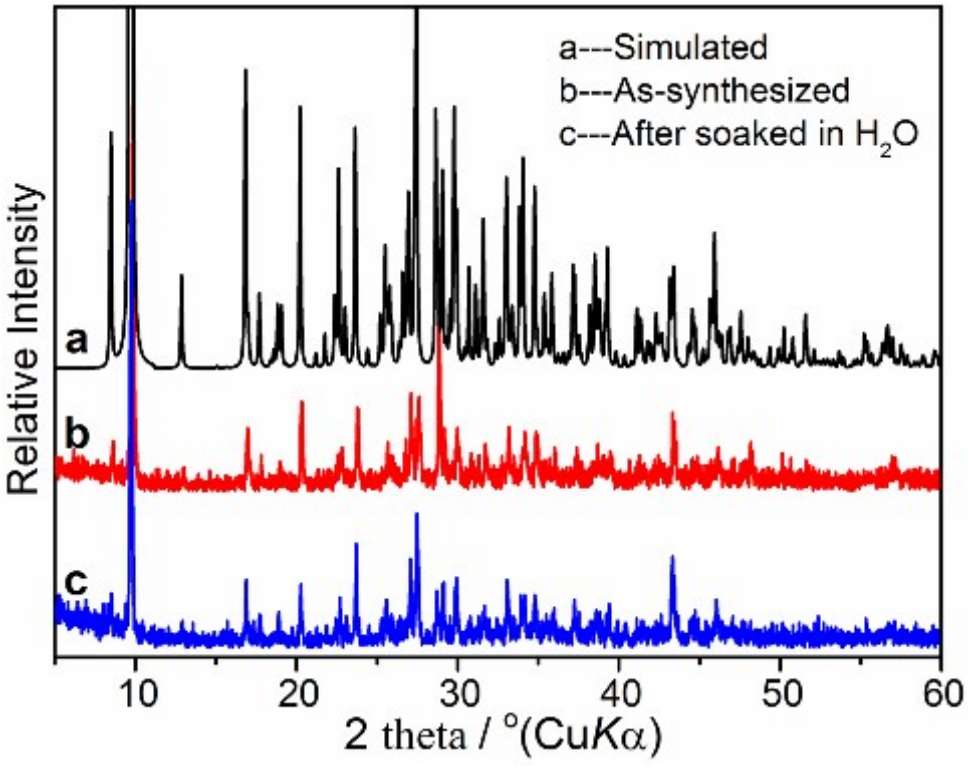
Symmetry transformations used to generate equivalent atoms: #1 x, -y+1/2, z-1/2; #2 x,-y+1/2,z+1/2; #3 -x+1,-y+1,-z.



(a)



(b)



(c)

Fig. S1 The PXRD patterns of **3** (a), **5** (b), and **6** (c) under different conditions.

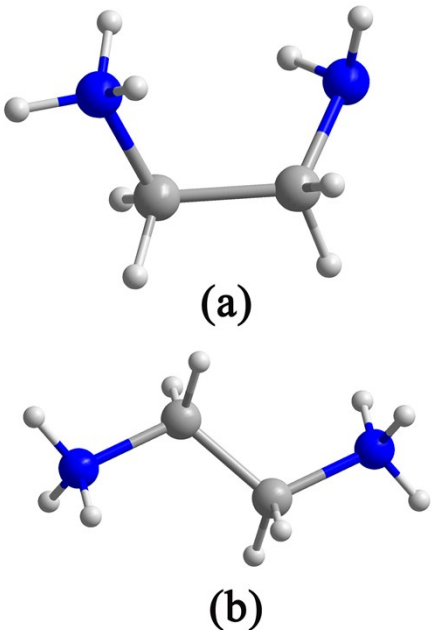
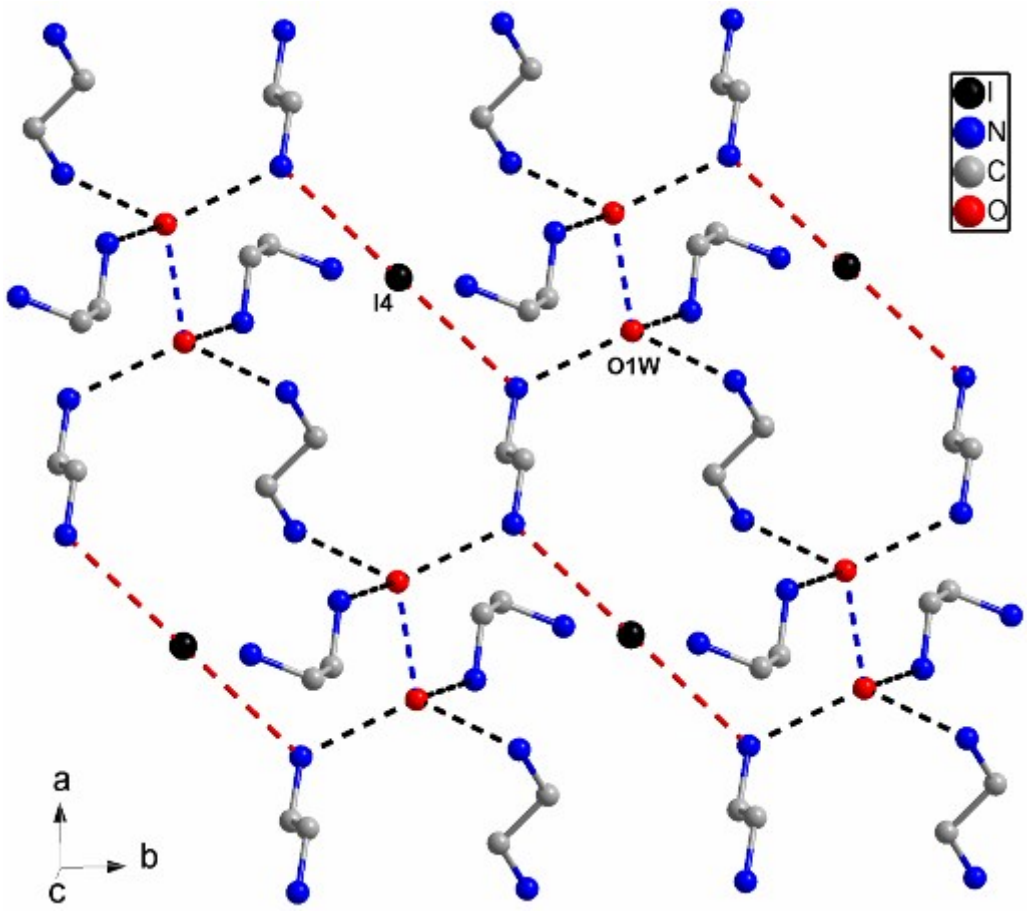
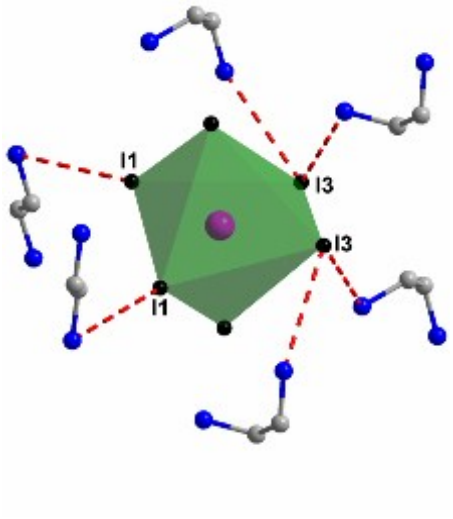


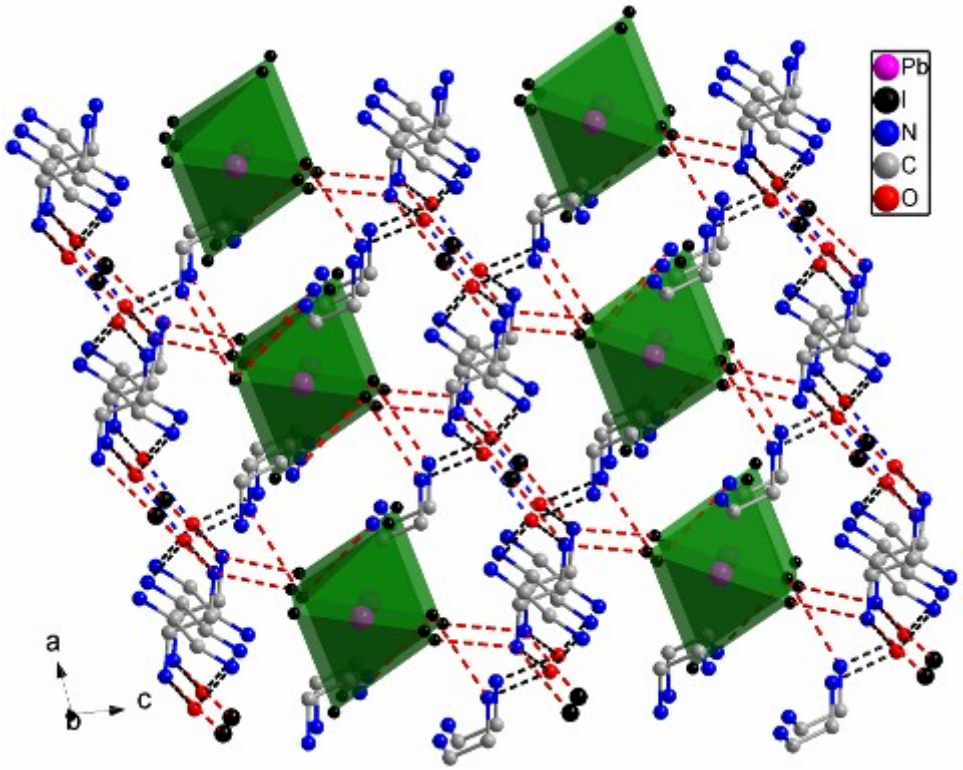
Fig. S2 The protonated en molecules with two different configurations observed in the structure of **1**.



(a)



(b)



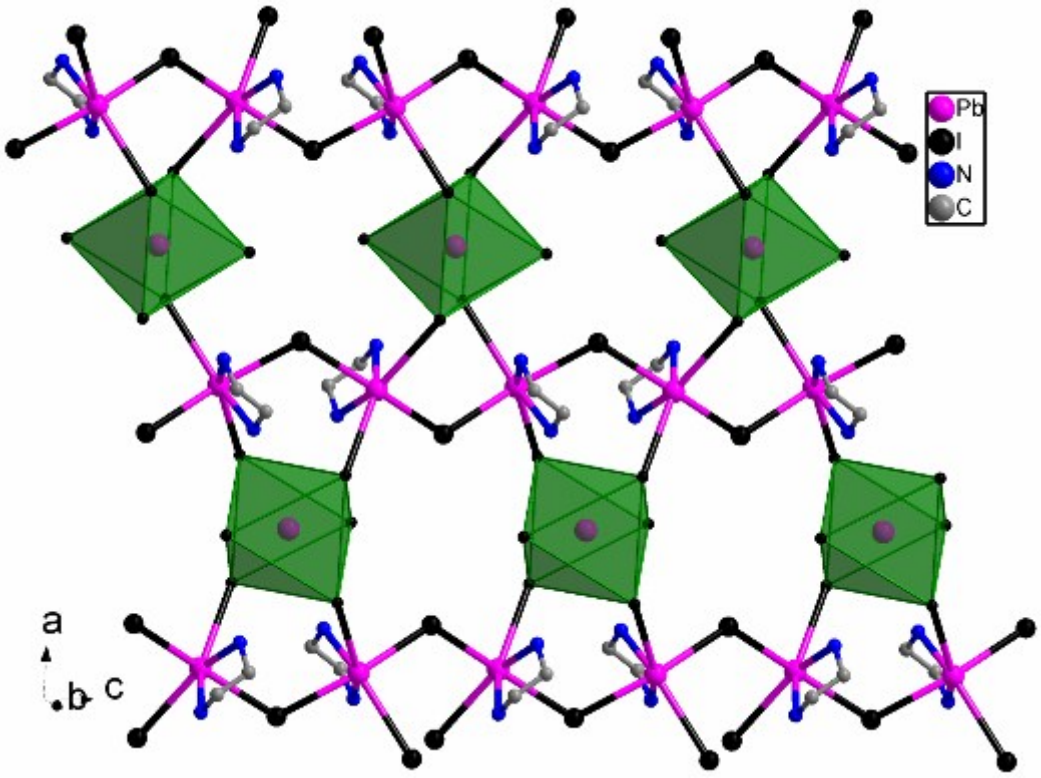
(c)

Fig. S3 (a) The 2-D supramolecular layer formed by I^- ion, protonated en and H_2O molecules through N-H···I (red dashed lines), N-H···O (black dashed lines), and O-H···O (blue dashed lines) hydrogen bonds. (b) The hydrogen bonds around a (PbI_6) octahedron. (c) Polyhedral view of the 3-D supramolecular framework of **1** along the *b* axis. Hydrogen atoms are omitted for clarity. Green octahedron: (PbI_6).

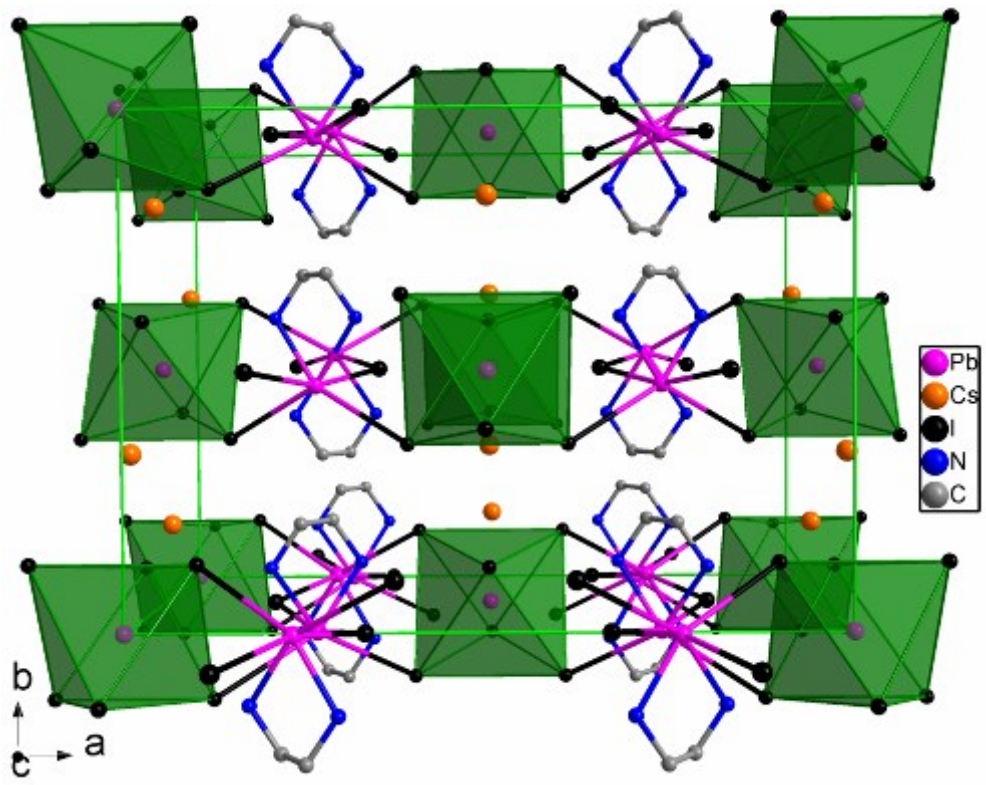
Table S2. Selected Hydrogen Bonds Data for **1**.

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	∠(DHA) (°)
N1-H1C···I4	0.89	2.97	3.724(3)	144.1
N1-H1A···I1[a]	0.89	3.07	3.795(4)	139.5
N1-H1B···O1W[b]	0.89	2.06	2.784(4)	138.1
N3-H3E···I3[c]	0.89	3.03	3.659(4)	129.5
N4-H4B···O1W[d]	0.89	1.95	2.798(4)	157.7
O1W-H1I···N4[d]	0.85	2.22	2.798(4)	125.6
N2-H2A···I3[e]	0.89	2.74	3.594(4)	161.9
O1W-H1H···O1W[f]	0.82	2.27	2.726(5)	115.4
O1W-H1F···N3[g]	0.82	1.91	2.704(5)	163.2
O1W-H1G···N1[h]	0.82	2.02	2.784(4)	154.0

Symmetry codes: a (1/2-x, -1/2+y, 3/2-z); b (-1/2+x, 1/2+y, z); c (1-x, y, 3/2-z); d (1-x, 1-y, 1-z); e (-1/2+x, 1/2+y, z); f (3/2-x, 1/2-y, 1-z); g (1-x, y, 3/2-z); h (1/2+x, -1/2+y, z).



(a)



(b)

Fig. S4 (a) Polyhedral view of the hybrid 2-D layer structure of **2**. (b) Crystal packing diagram of **2**. Hydrogen atoms are omitted for clarity. Green octahedron: (PbI_6).

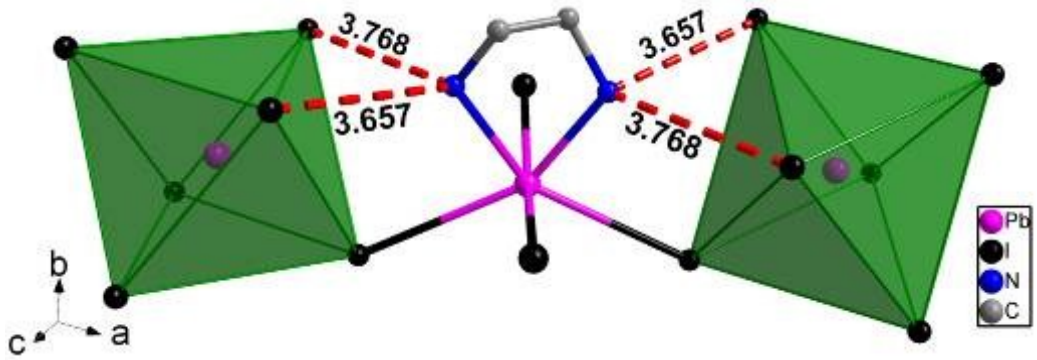
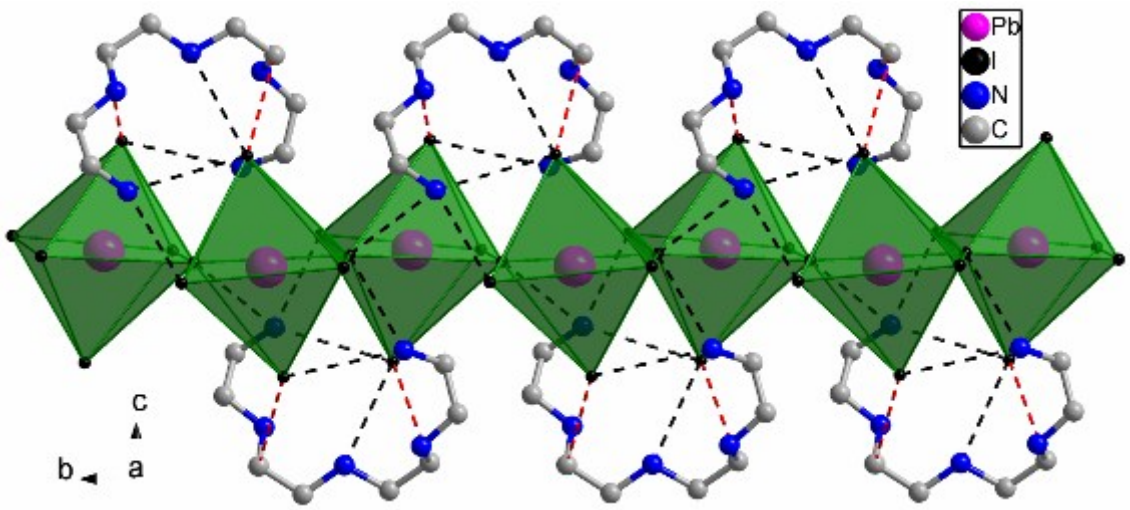


Fig. S5 View of the N-H···I (red dashed lines) hydrogen bonds within the 2-D layer of **2**.

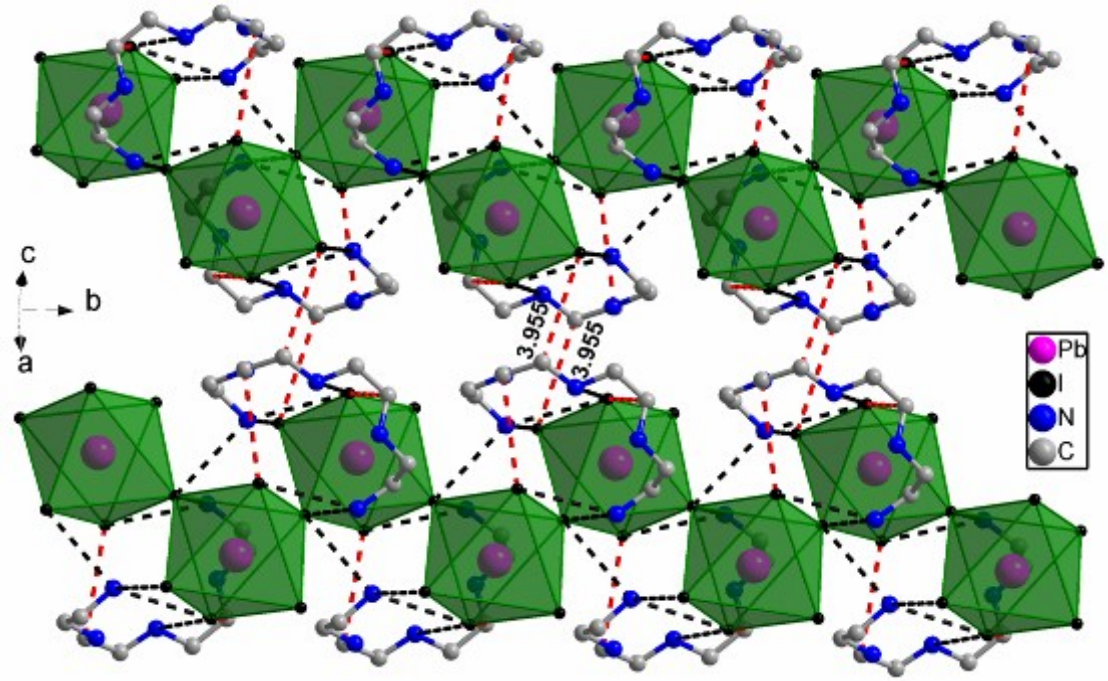
Table S3. Selected Hydrogen Bonds Data for **2**.

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	∠(DHA) (°)
N1-H11A...I1[a]	0.90	2.80	3.658(4)	159.3
N1-H11B...I2[b]	0.90	2.99	3.768(3)	145.5

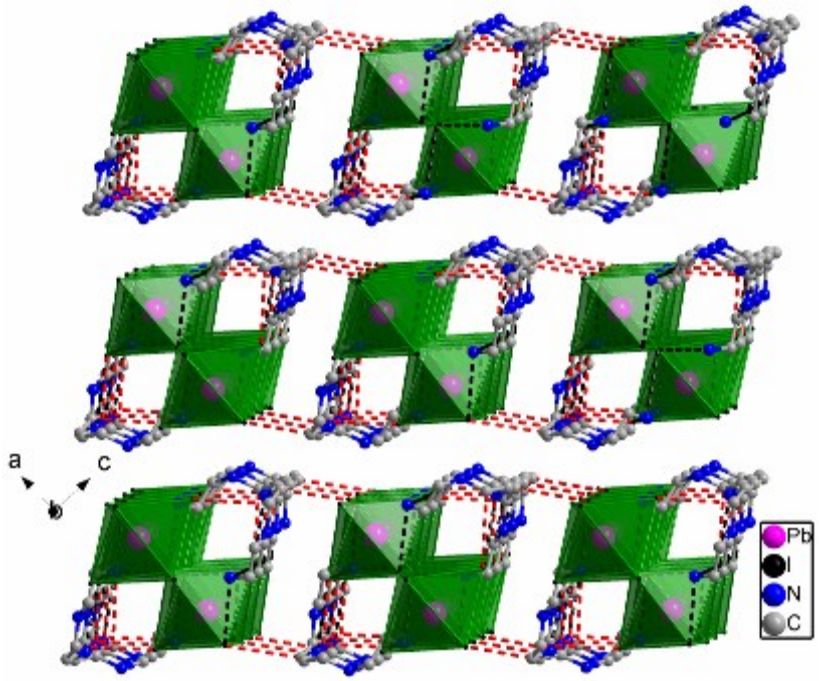
Symmetry codes: a (x, y, -1+z); b (x, 1-y, 1-z).



(a)



(b)



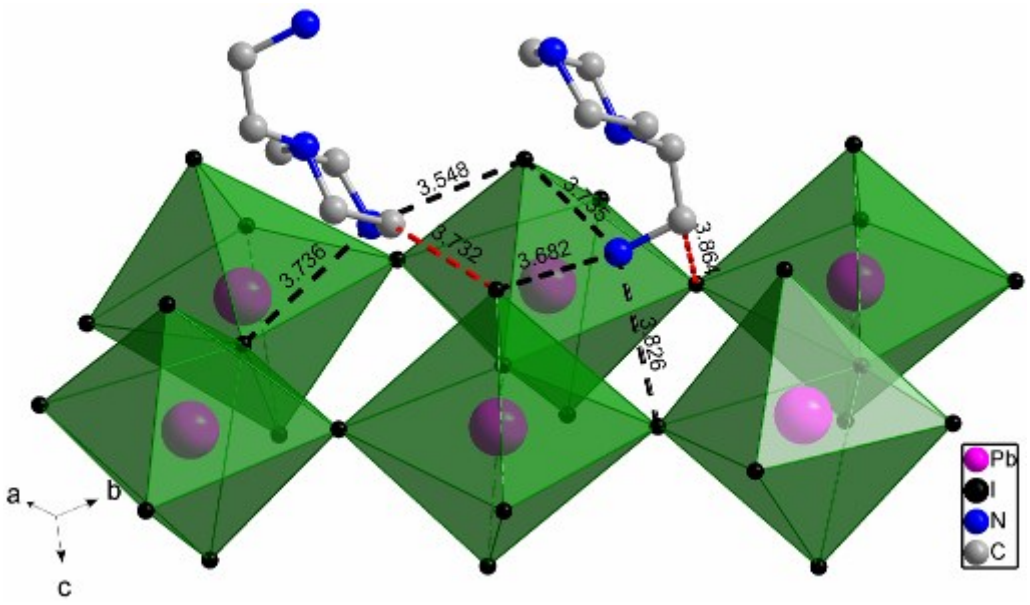
(c)

Fig. S6 (a) The 1-D supramolecular hybrid chain formed by 1-D inorganic $(PbI_5)^{3-}$ anionic chain and $(H_3tepa)^{3+}$ cation. (b) The 2-D supramolecular layer in **3** parallel to the (101) plane. (c) Polyhedral view of the 3-D supramolecular framework of **3** along the *b* axis. The hydrogen atoms are omitted for clarity.

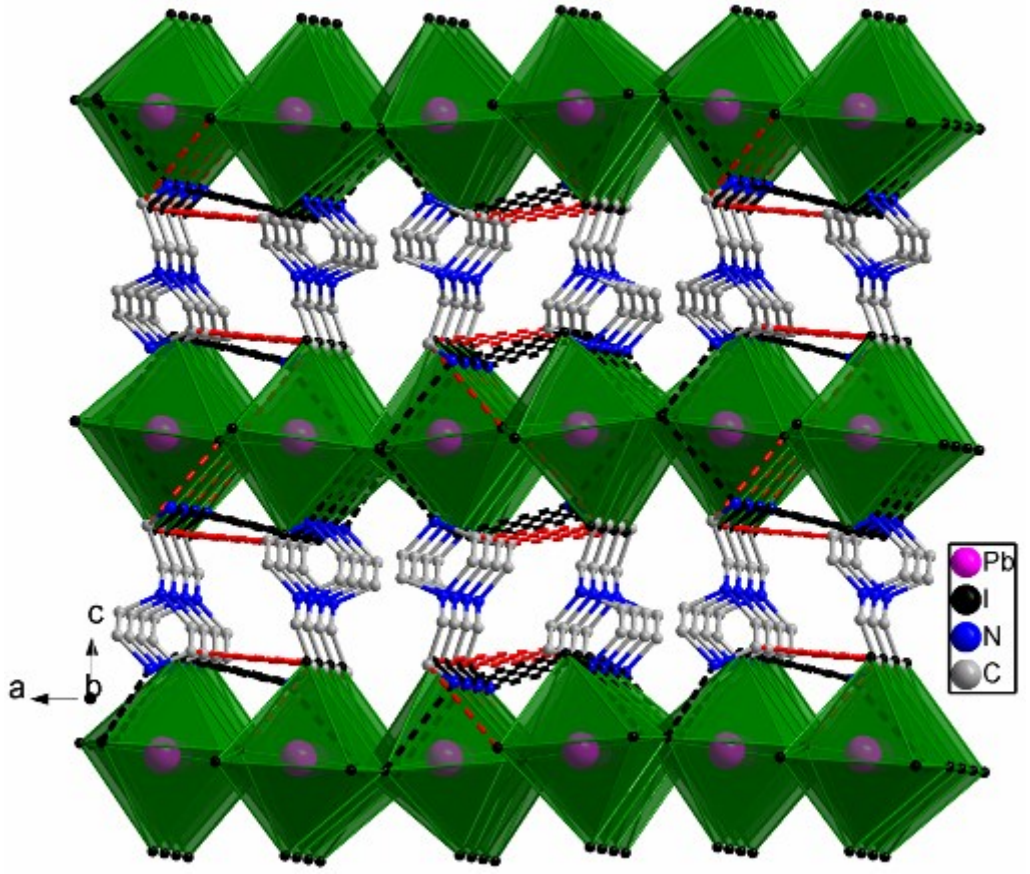
Table S4. Selected Hydrogen Bonds Data for **3**.

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	∠(DHA) (°)
C4–H4A···I4	0.97	3.01	3.955(4)	164.9
N5–H11C···I1[a]	0.89	2.89	3.673(3)	148.2
N3–H11B···I3 [a]	0.90	3.08	3.902(3)	152.6
C6–H6A···I3[a]	0.97	3.07	3.925(4)	147.6
N1–H12C···I3[a]	0.89	2.78	3.576(3)	149.8
N1–H12A···I4[a]	0.89	2.82	3.685(3)	166.0
N5–H11D···I5[b]	0.89	2.76	3.540(3)	146.4
C3–H3A···I5[b]	0.97	3.09	3.891(4)	140.9
N1–H12B···I1[b]	0.89	2.86	3.550(3)	135.3

Symmetry codes: a (1-x, 1-y, 1-z); b (1/2+x, 1/2-y, -1/2+z).



(a)



(b)

Fig. S7 (a) View of the N–H···I (black dashed lines) and C–H···I (black dashed lines) hydrogen bonds of **4**. (b) Polyhedral view of the 3-D sandwich-like supramolecular framework of **4**.

Table S5. Selected Hydrogen Bonds Data for **4**.

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	∠(DHA) (°)
N1–H11A···I2	0.89	3.02	3.826(4)	151.7
N1–H11C···I1	0.89	2.89	3.682(3)	149.5
N1–H11B···I3[a]	0.89	2.90	3.735(4)	157.9
C6–H6B···I1[b]	0.97	3.00	3.938(5)	163.9
C1–H1A···I1[c]	0.97	3.10	3.732(4)	124.3
N3–H12A···I3[d]	0.90	2.82	3.548(4)	138.4
N3–H12B···I2[e]	0.90	2.86	3.736(3)	164.4

Symmetry codes: a (-x, 1/2+y, 1/2-z); b (1/2-x, 1/2+y, z); c (-x, 1-y, 1-z); d (x, 1/2-y, 1/2+z); e (x, 3/2-y, 1/2+z).

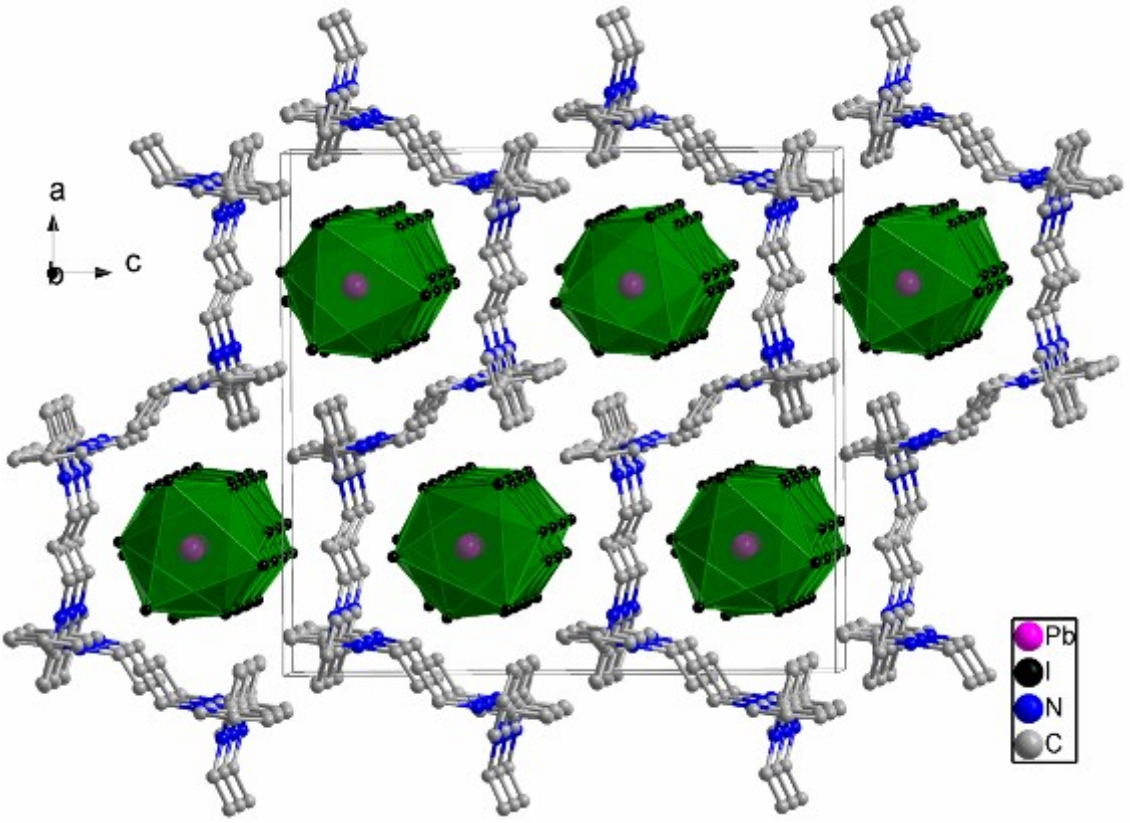


Fig. S8 Polyhedral view of the 3-D packing diagram of **5** along the *b* direction.

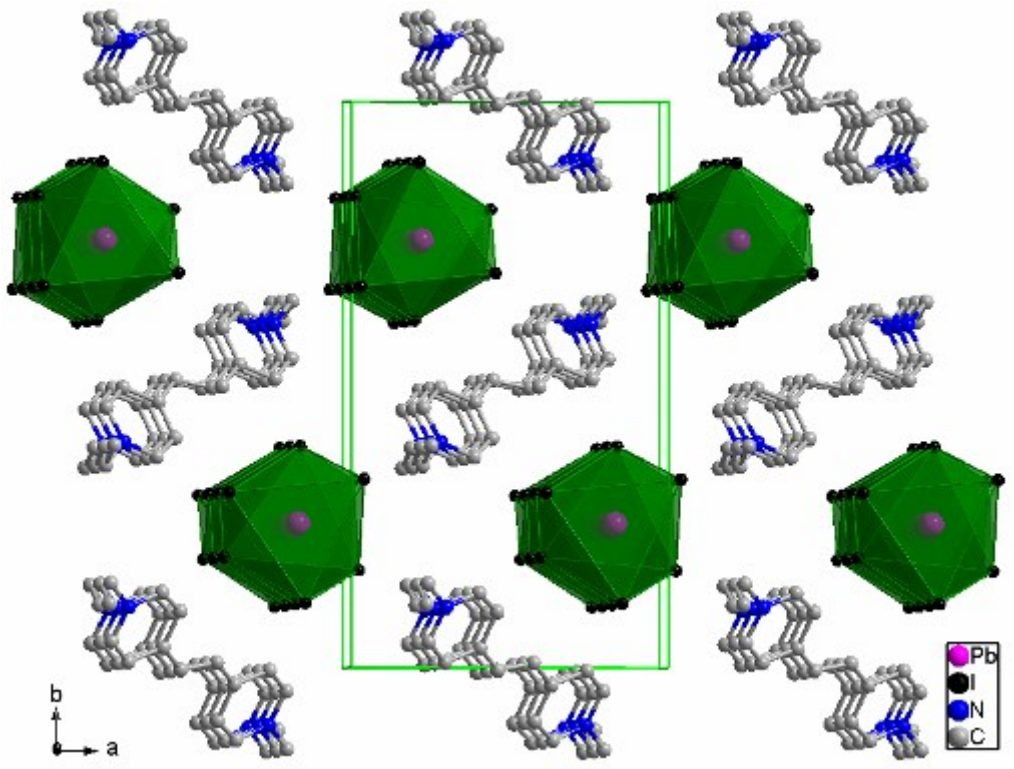


Fig. S9 Polyhedral view of the 3-D packing diagram of **6** along the *c* direction.

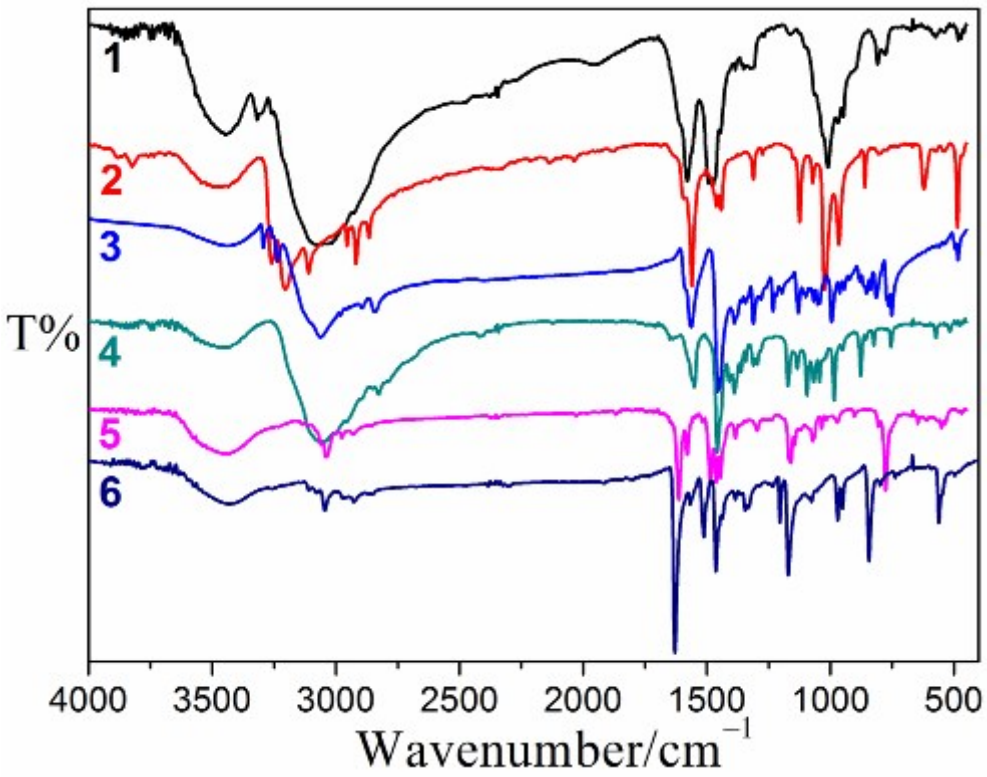
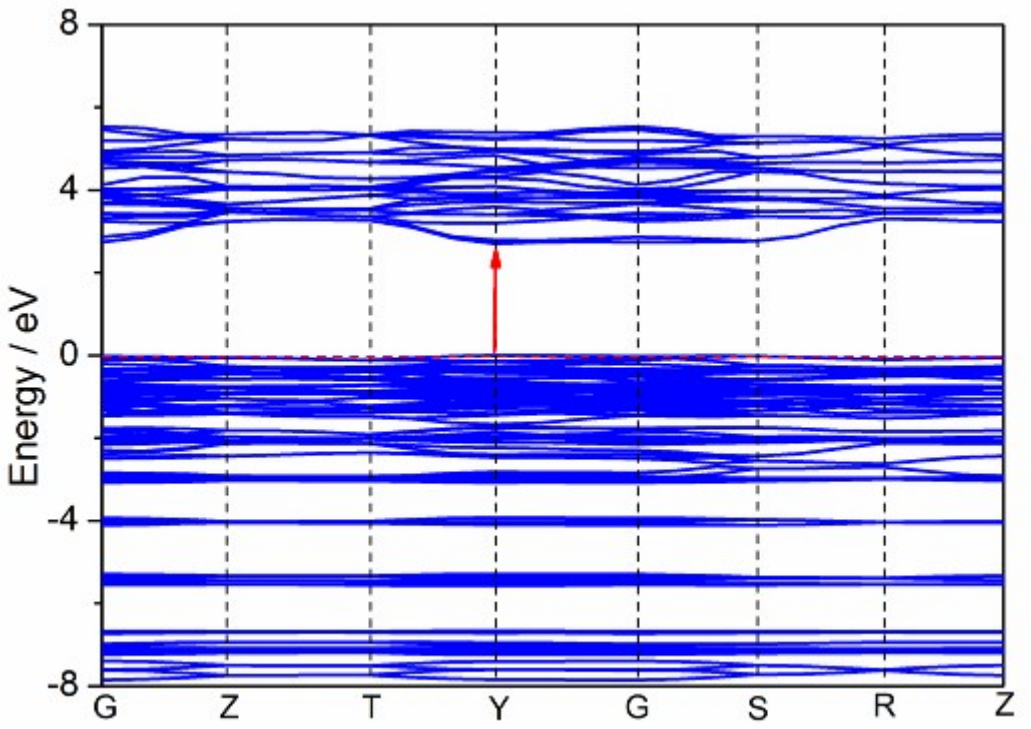
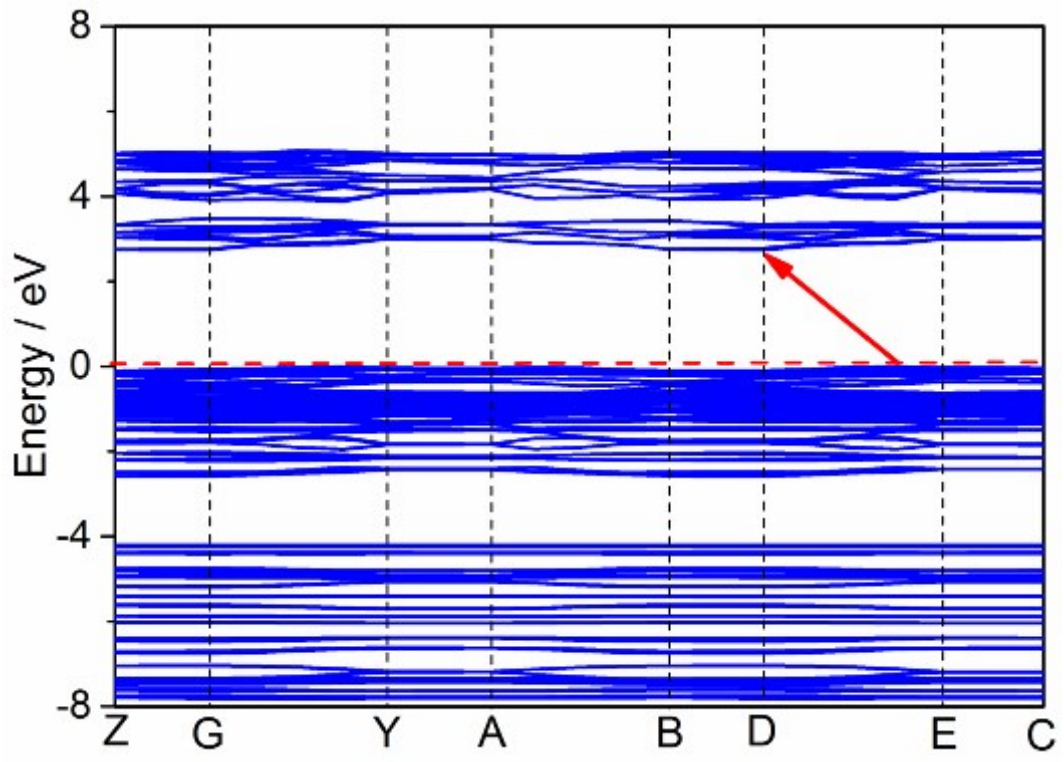


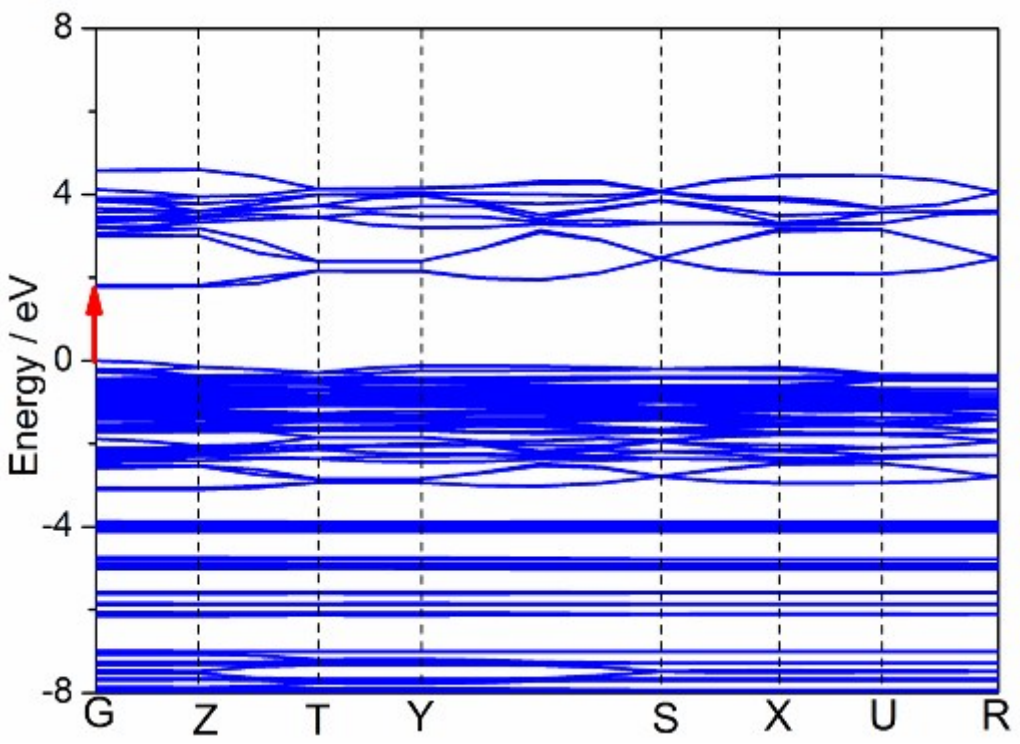
Fig. S10 IR spectra of **1**–**6**.



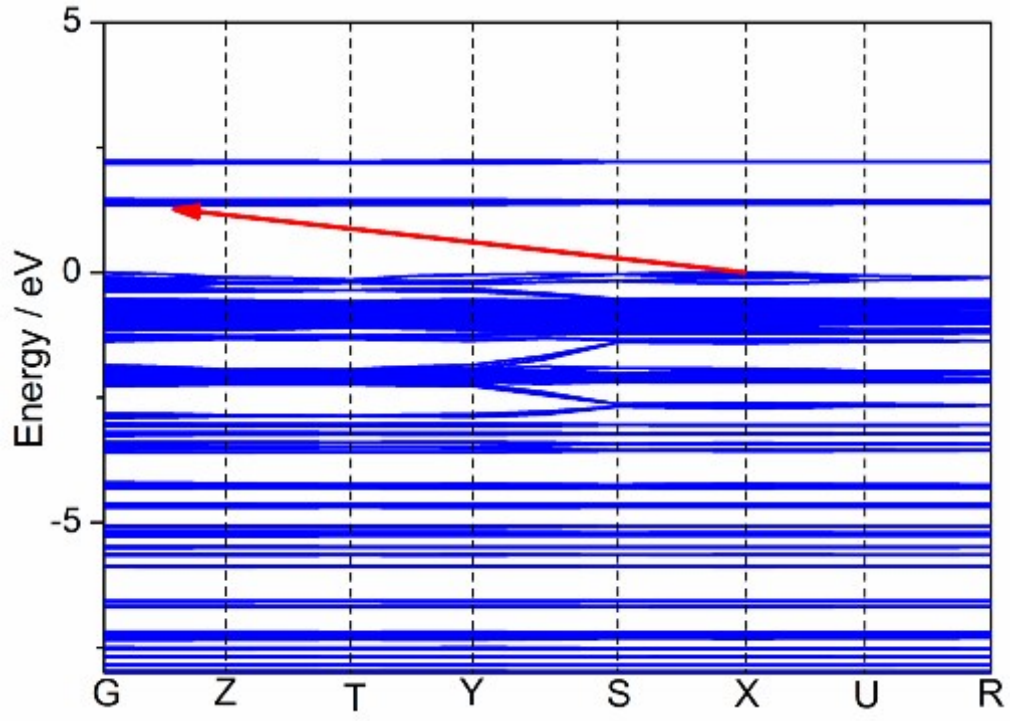
(a)



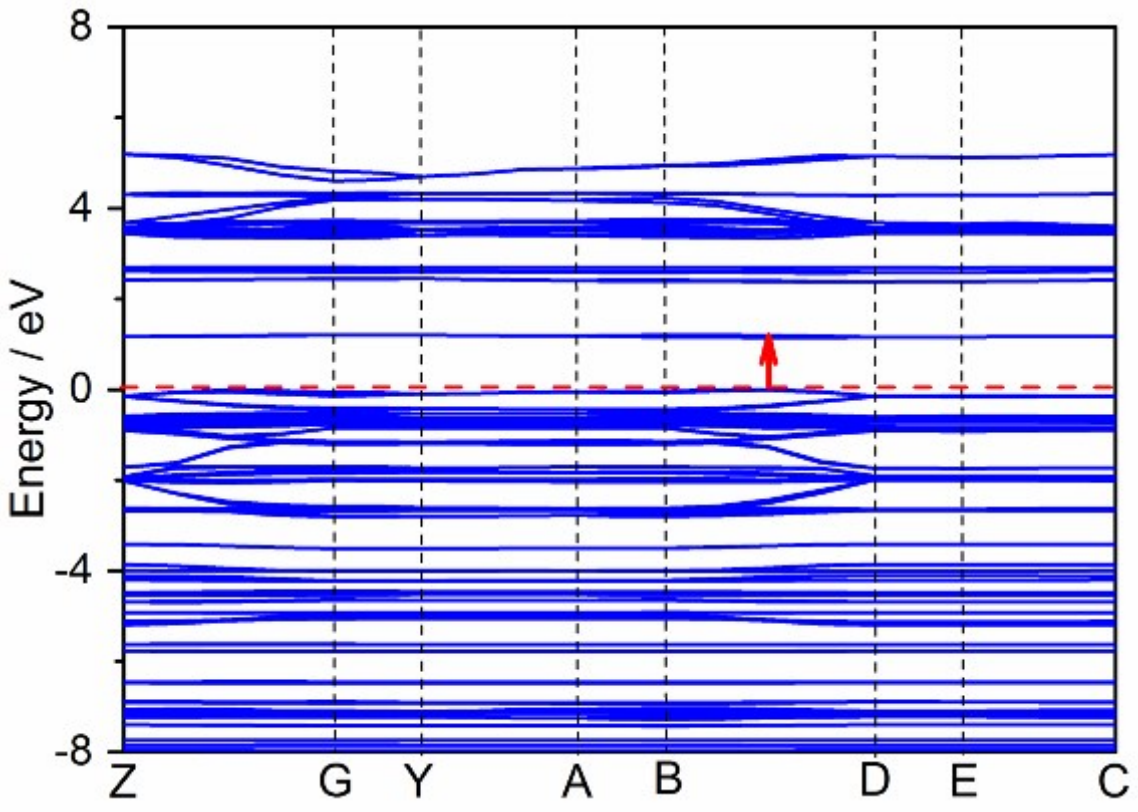
(b)



(c)



(d)



(e)

Fig. S11 Band structures of **2** (a), **3** (b), **4** (c), **5** (d), and **6** (e). The Fermi level is set at 0 eV.

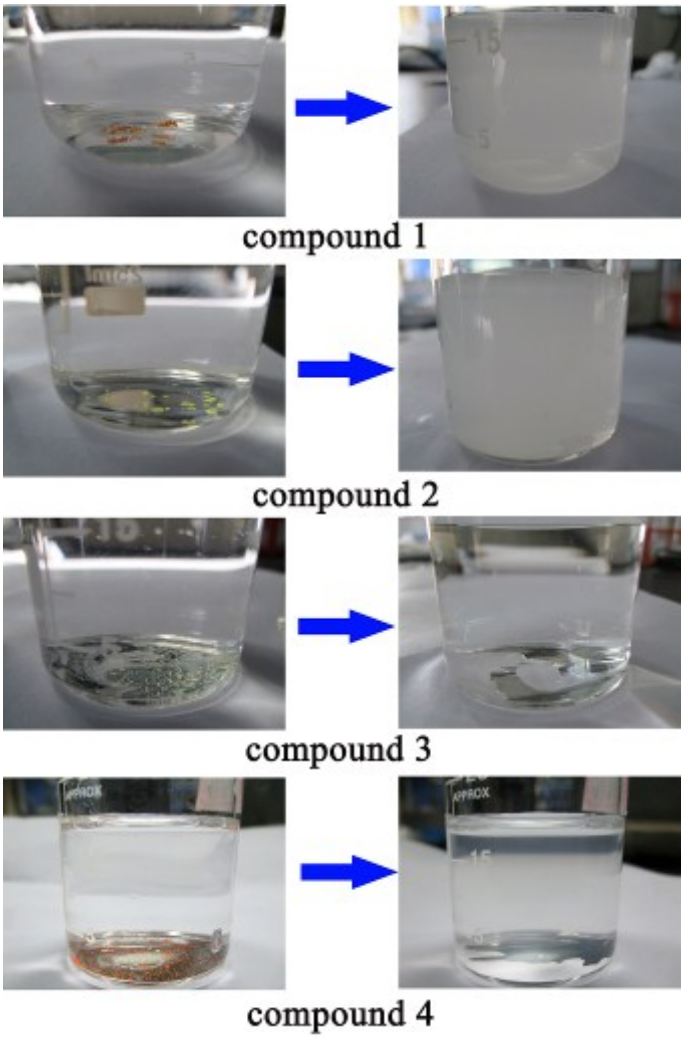


Fig. S12 6 mg sample in 20 mL water before and after ultrasonic treatment.

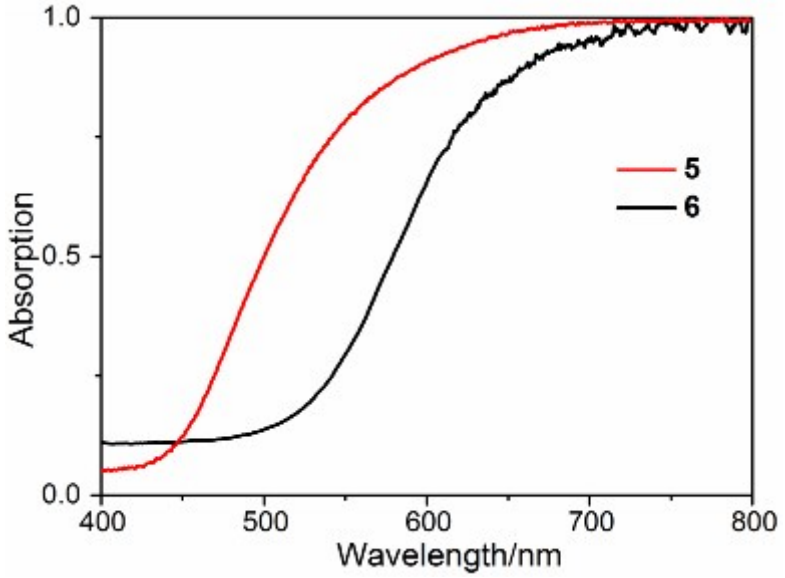
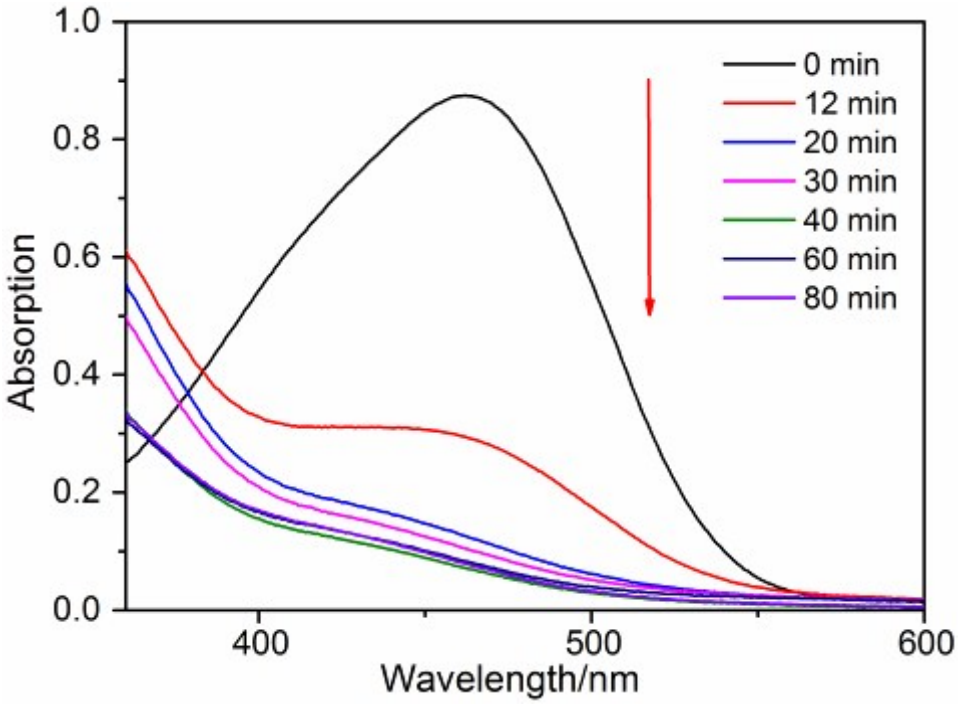
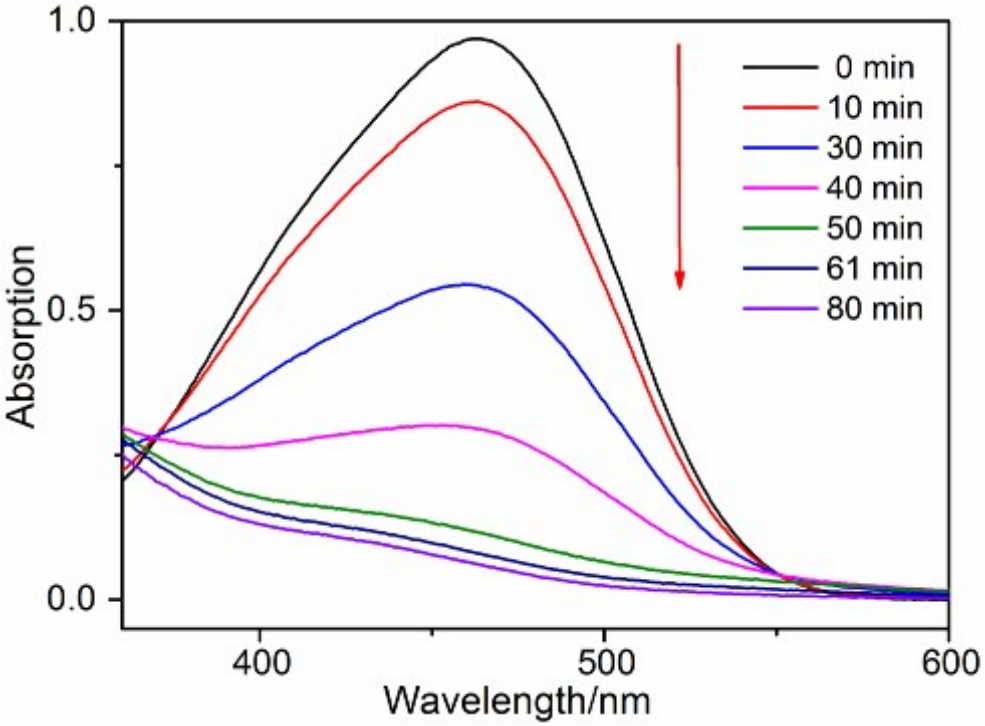


Fig. S13 The absorption spectra of **5** and **6** in the visible light.

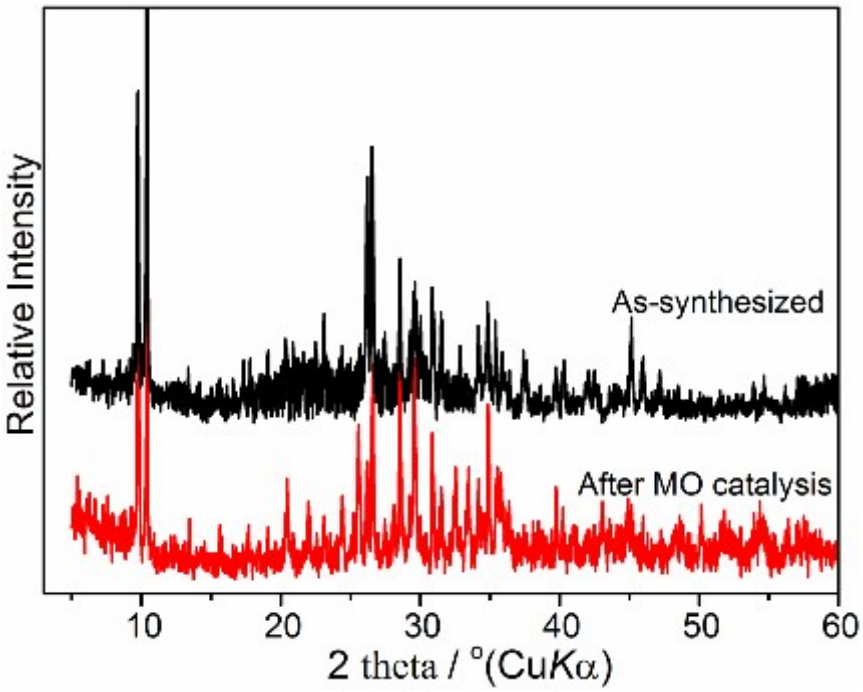


(a)

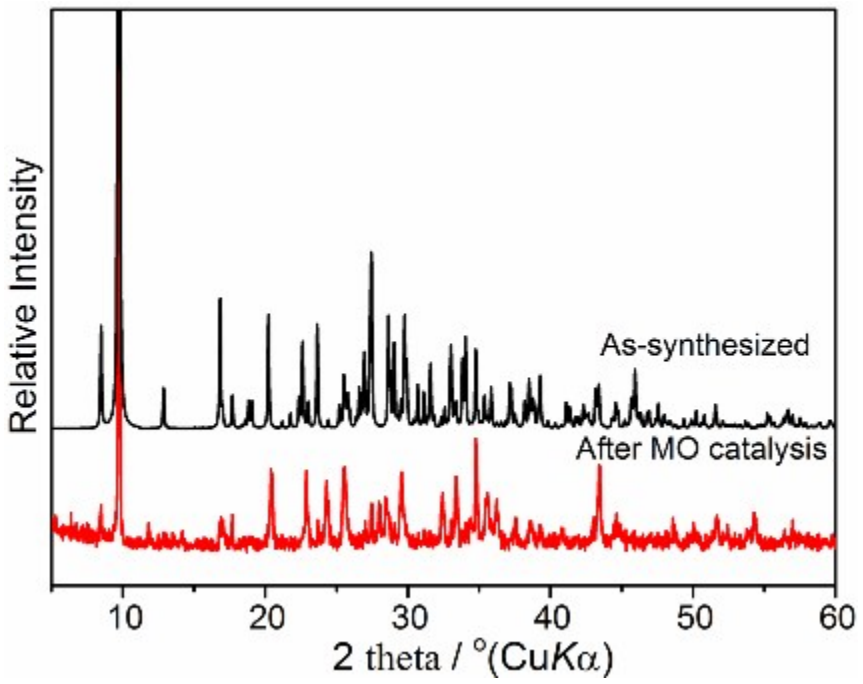


(b)

Fig. S14 Time-dependent UV/vis spectra of MO over **5** (a) and **6** (b).



(a)



(b)

Fig. S15 The PXRD patterns of **5** (a), and **6** (b) after visible light photocatalysis. The slight peak changes from 25 to 35 degree for both samples after photodegradation experiments might be due to the structural distortion.

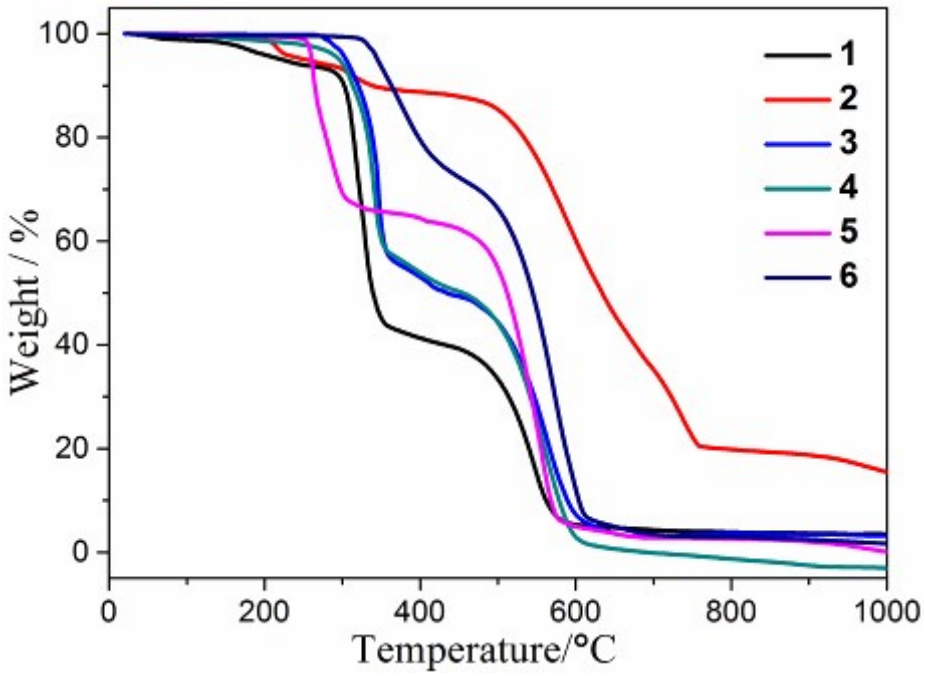


Fig. S16 TGA curves of **1**–**6**.