Electronic Supplementary Information for

Syntheses and properties of 2-D and 3-D heterometallic Pb–Ag iodometallates decorated by ethylene polyamines at Pb(II) center

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Table S1. Selected Bond Lengths (Å) and Angles (deg) for **1**

Ag(1)–I(1)	2.8871(12)	Ag(1)–I(1)#1	2.8572(11)
Ag(1)–I(2)	2.8077(11)	Ag(1)–I(3)	2.8356(13)
Ag(1)–Ag(1)#1	3.0244(18)	Pb(1)–I(2)	3.5498(11)
Pb(1)–I(2)#1	3.5457(11)	Pb(1)–I(2)	3.5504(11)
Pb(1)···I(1)#1	3.7518(11)	Pb(1)···I(1)	3.7602(11)
Pb(1)–N(1)	2.547(9)	Pb(1)–N(2)	2.557(9)
Pb(1)–N(3)	2.528(10)	Pb(1)–N(4)	2.563(9)
I(1)–Ag(1)–I(1)#1	116.46(3)	I(1)–Ag(1)–I(2)	103.29(4)
I(1)#1–Ag(1)–I(2)	112.38(4)	I(1)–Ag(1)–I(3)	110.12(4)
I(1)#1–Ag(1)–I(3)	105.98(4)	I(2)–Ag(1)–I(3)	108.47(4)
I(2)–Pb(1)–N(1)	79.9(2)	I(2)–Pb(1)–N(2)	140.4(2)
I(2)–Pb(1)–N(3)	139.6(2)	I(2)–Pb(1)–N(4)	79.3(2)
I(2)#1–Pb(1)–N(1)	139.0(2)	I(2)#1–Pb(1)–N(2)	78.1(2)
I(2)#1–Pb(1)–N(3)	78.5(2)	I(2 #1–Pb(1)–N(4)	140.0(2)
N(1)–Pb(1)–N(2)	67.4(3)	N(1)–Pb(1)–N(3)	112.2(3)
N(1)–Pb(1)–N(4)	76.1(3)	N(2)–Pb(1)–N(3)	76.0(3)
N(2)–Pb(1)–N(4)	112.0(3)	N(3)–Pb(1)–N(4)	67.6(3)
Ag(1)–I(1)–Ag(1)#1	63.54(3)	Ag(1)–I(2)–Pb(1)	113.42(3)

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

Table S1. Selected Bond Lengths (Å) and Angles (deg) for **2**

Ag(1)–I(1)	2.863(3)	Ag(1)–I(1)#1	2.874(3)
Ag(1)–I(2)	2.861(3)	Ag(1)–I(3)	2.818(3)
Pb(1)–I(2)	3.466(3)	Pb(1)–I(2)#1	3.619(3)
Pb(1)···I2(1)	3.672(3)	Pb(1)···I3(1)	4.187(3)
Ag(1)···Ag(1)#1	3.639(3)		
Pb(1)–N(1)	2.60(3)	Pb(1)–N(2)	2.41(2)
Pb(1)–N(3)	2.53(3)	Pb(1)–N(4)	2.58(2)
I(1)–Ag(1)–I(1)#1	101.28(9)	I(1)–Ag(1)–I(2)	107.24(10)
I(1)#1–Ag(1)–I(2)	106.86(10)	I(1)–Ag(1)–I(3)	116.53(11)
I(1)#1–Ag(1)–I(3)	114.98(10)	I(2)–Ag(1)–I(3)	109.22(10)
N(1)–Pb(1)–N(3)	75.1(8)	N(1)–Pb(1)–N(2)	70.4(8)
N(2)–Pb(1)–N(3)	83.6(9)	N(1)–Pb(1)–N(4)	136.4(8)
N(3)–Pb(1)–N(4)	66.7(7)	N(2)–Pb(1)–N(4)	84.9(8)
N(1)–Pb(1)–I(2)	77.1(8)	N(2)–Pb(1)–I(2)	145.0(8)
N(3)–Pb(1)–I(2)	75.2(9)	N(4)–Pb(1)–I(2)	110.8(9)
Ag(1)–I(1)–Ag(1)#1	78.72(9)		

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

Table S3. Selected Bond Lengths (Å) and angles (deg) for **3**

Ag(1)–I(3)	2.833(2)	Ag(1)–I(2)	2.857(3)
Ag(1)–I(1)	2.890(3)	Ag(1)–I(1)#1	2.872(3)
Ag(1)···Ag(1)#1	3.788(3)	Ag(1)···Pb(1)	4.162(3)
Pb(1)–I(3)	3.3794(17)	Pb(1)–I(3)#2	3.3728(16)
Pb(1)–I(2)	3.1103(18)	Pb(1)–I(1)#2	3.4141(17)
Pb(1)–N(1)	2.537(17)	Pb(1)–N(2)	2.55(2)
I(3)–Ag(1)–I(2)	102.13(7)	I(3)–Ag(1)–I(1)	107.30(8)
I(3)–Ag(1)–I(1)#1	116.08(9)	I(2)–Ag(1)–I(1)	118.79(9)
I(2)–Ag(1)–I(1)#1	115.26(9)	I(1)–Ag(1)–I(1)#1	97.80(7)
I(3)–Pb(1)–I(3)#2	118.32(3)	I(3)–Pb(1)–I(2)	85.88(4)
I(3)#2–Pb(1)–I(2)	90.00(5)	I(3)–Pb(1)–I(1)#2	86.11(4)
I(3)#2–Pb(1)–I(1)#2	85.56(4)	I(2)–Pb(1)–I(1)#2	167.66(5)
N(1)–Pb(1)–N(2)	72.3(8)	N(1)–Pb(1)–I(3)	85.7(6)
N(1)–Pb(1)–I(3)#2	155.9(6)	N(1)–Pb(1)–I(2)	94.0(6)

N(1)–Pb(1)–I(1)#2	94.7(6)	N(2)–Pb(1)–I(3)	157.7(5)
N(2)–Pb(1)–I(3)#2	83.8(5)	N(2)–Pb(1)–I(2)	92.0(5)
N(2)–Pb(1)–I(1)#2	98.9(5)	Ag(1)–I(3)–Pb(1)	83.63(6)
Ag(1)–I(3)–Pb(1)#3	84.34(5)	Pb(1)–I(3)–Pb(1)#3	125.25(5)
Ag(1)–I(2)–Pb(1)	88.34(6)	Ag(1)#1–I(1)–Ag(1)	82.20(7)
Ag(1)–I(1)–Pb(1)#3	82.74(6)	Ag(1)#1–I(1)–Pb(1)#3	116.84(7)

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

Table S4. Selected Bond Lengths (Å) and angles (deg) for **4**

Ag(1)–I(1)	2.8821(18)	Ag(1)–I(1)#1	2.8892(18)
Ag(1)–I(2)	2.799(2)	Ag(1)–I(3)	2.8473(17)
Pb(1)–I(3)	3.470(3)	Pb(1)–I(3)#1	3.572(3)
Pb(1)···I(1)	3.672(3)	Ag(1)–Ag(1)#1	3.106(3)
Pb(1)–N(2)	2.554(15)	Pb(1)–N(1)	2.538(15)
Pb(1)–N(4)	2.509(15)	Pb(1)–N(3)	2.589(16)
I(1)–Ag(1)–I(1)#1	114.89(6)	I(1)–Ag(1)–I(2)	110.64(6)
I(1)#1–Ag(1)–I(2)	114.90(6)	I(1)–Ag(1)–I(3)	106.16(6)
I(1)#1–Ag(1)–I(3)	99.84(5)	I(2)–Ag(1)–I(3)	109.38(6)
Ag(1)#1–Ag(1)–I(1)	57.55(5)	Ag(1)#1–Ag(1)–I(1)#1	57.33(5)
Ag(1)#1–Ag(1)–I(2)	135.96(8)	Ag(1)#1–Ag(1)–I(3)	114.66(8)
N(1)–Pb(1)–N(3)	108.0(5)	N(1)–Pb(1)–N(2)	68.0(5)
N(2)–Pb(1)–N(3)	68.2(5)	N(1)–Pb(1)–N(4)	77.9(5)
N(3)–Pb(1)–N(4)	69.3(5)	N(2)–Pb(1)–N(4)	111.8(5)
N(1)–Pb(1)–I(3)	80.0(5)	N(2)–Pb(1)–I(3)	144.3(5)
N(3)–Pb(1)–I(3)	142.9(5)	N(4)–Pb(1)–I(3)	78.7(5)
Ag(1)–I(1)–Ag(1)#1	65.11(6)		

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

Table S5. Selected Bond Lengths (Å) and angles (deg) for **5**

Ag(1)–I(1)	2.866(2)	Ag(1)–I(2)	2.866(2)
Ag(1)–I(3)	2.884(2)	Ag(1)–I(4)	2.877(2)
Ag(2)–I(1)#1	2.878(2)	Ag(2)–I(2)#1	2.878(2)
Ag(2)–I(3)	2.874(2)	Ag(2)–I(4)	2.878(2)
Pb(1)–I(2)	3.572(3)	Pb(1)–I(4)	3.6750(16)
Pb(1)···I(1)	3.953(3)		
Ag(1)···Ag(2)	3.137(3)	Ag(1)···Ag(2)#1	3.724 (3)
Pb(1)–N(1)	2.683(13)	Pb(1)–N(2)	2.539(17)
Pb(1)–N(3)	2.616(18)	Pb(1)–N(4)	2.621(14)
Pb(1)–N(5)	2.544(14)		
I(1)–Ag(1)–I(2)	98.58(6)	I(1)–Ag(1)–I(3)	113.65(8)
I(1)–Ag(1)–I(4)	117.75(7)	I(2)–Ag(1)–I(3)	108.76(7)
I(2)–Ag(1)–I(4)	113.83(8)	I(3)–Ag(1)–I(4)	104.29(6)
I(1)#1–Ag(2)–I(2)#1	98.02(6)	I(1)#1–Ag(2)–I(3)	119.85(8)
I(1)#1–Ag(2)–I(4)	111.70(8)	I(2)#1–Ag(2)–I(3)	109.90(8)
I(2)#1–Ag(2)–I(4)	113.09(7)	I(3)–Ag(2)–I(4)	104.52(7)
N(1)–Pb(1)–N(2)	66.2(6)	N(1)–Pb(1)–N(3)	133.4(6)
N(1)–Pb(1)–N(4)	137.9(6)	N(1)–Pb(1)–N(5)	72.2(5)
N(2)–Pb(1)–N(3)	68.4(5)	N(2)–Pb(1)–N(4)	107.0(5)
N(2)–Pb(1)–N(5)	80.2(6)	N(3)–Pb(1)–N(4)	66.7(5)
N(3)–Pb(1)–N(5)	110.0(5)	N(4)–Pb(1)–N(5)	65.7(5)
N(1)–Pb(1)–I(4)	75.3(4)	N(2)–Pb(1)–I(4)	137.9(4)
N(3)–Pb(1)–I(4)	151.2(4)	N(4)–Pb(1)–I(4)	90.2(4)
N(5)–Pb(1)–I(4)	72.3(4)	N(1)–Pb(1)–I(2)	74.9(4)
N(2)–Pb(1)–I(2)	81.5(4)	N(3)–Pb(1)–I(2)	88.5(4)
N(4)–Pb(1)–I(2)	147.0(4)	N(5)–Pb(1)–I(2)	146.7(4)
Ag(1)–I(2)–Ag(2)#2	80.81(6)	Ag(1)–I(1)–Ag(2)#2	80.83(6)
Ag(1)–I(4)–Ag(2)	66.05(6)	Ag(1)–I(3)–Ag(2)	66.02(6)
Ag(2)–I(4)–Pb(1)	114.74(6)	Ag(1)–I(4)–Pb(1)	126.86(6)

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

Table S6. Selected Bond Lengths (Å) and angles (deg) for **6**

Ag(1)–I(1)	2.9737(18)	Ag(1)–I(2)	2.8329(19)
Ag(1)–I(3)	2.824(2)	Ag(1)–I(4)#1	2.7993(17)
Ag(2)–I(1)	2.9828(18)	Ag(2)–I(2)	2.7989(17)
Ag(2)–I(4)	2.8279(19)	Ag(2)–I(5)	2.821(2)
Ag(3)–I(3)	2.8298(16)	Ag(3)–I(6)	2.772(4)
Ag(4)–I(5)	2.8475(17)	Ag(4)–I(7)	2.761(4)
Ag(1)···Ag(2)#1	3.424(4)	Ag(1)···Ag(2)	3.431(4)
Pb(1)–I(2)	3.5784(14)	Pb(1)···I(5)#1	3.9230(11)
Pb(1)–I(5)	3.6311(11)		
Pb(2)–I(3)	3.6086(12)	Pb(2)–I(4)	3.6112(15)
Pb(1)–N(1)	2.533(12)	Pb(1)–N(2)	2.468(11)
Pb(1)–N(3)	2.618(16)	Pb(2)–N(6)	2.557(12)
Pb(2)–N(4)	2.626(17)	Pb(2)–N(5)	2.487(12)
Pb(1)–O(1)	2.374(9)	Pb(2)–O(2)	2.356(8)
I(1)–Ag(1)–I(2)	106.42(7)	I(1)–Ag(1)–I(3)	101.92(7)
I(1)–Ag(1)–I(4) #1	107.03(6)	I(2)–Ag(1)–I(3)	108.14(6)
I(2)–Ag(1)–I(4)	112.92(7)	I(3)–Ag(1)–I(4) #1	119.13(7)
I(1)–Ag(2)–I(2)	107.07(6)	I(1)–Ag(2)–I(4)	106.04(7)
I(1)–Ag(2)–I(5)	101.66(7)	I(2)–Ag(2)–I(4)	112.78(6)
I(2)–Ag(2)–I(5)	119.05(7)	I(4)–Ag(2)–I(5)	108.87(6)
I(3)–Ag(3)–I(3)#1	104.55(7)	I(3)–Ag(3)–I(6)	114.03(6)
I(5)–Ag(4)–I(5)#2	103.77(7)	I(5)–Ag(4)–I(7)	114.70(6)
N(1)–Pb(1)–N(2)	70.4(5)	N(1)–Pb(1)–N(3)	138.5(4)
N(2)–Pb(1)–N(3)	69.0(4)	O(1)–Pb(1)–N(1)	76.3(4)
O(1)–Pb(1)–N(2)	78.2(4)	O(1)–Pb(1)–N(3)	87.3(5)
O(1)–Pb(1)–I(2)	97.0(3)	O(1)–Pb(1)–I(5)	139.2(2)
N(1)–Pb(1)–I(2)	73.1(3)	N(1)–Pb(1)–I(5)	138.5(3)
N(2)–Pb(1)–I(2)	143.2(3)	N(2)–Pb(1)–I(5)	126.7(3)
N(3)–Pb(1)–I(2)	147.7(3)	N(3)–Pb(1)–I(5)	75.9(3)
I(2)–Pb(1)–I(5)	80.30(3)	N(4)–Pb(2)–N(5)	67.8(4)
N(4)–Pb(2)–N(6)	137.2(4)	N(5)–Pb(2)–N(6)	70.2(4)
I(3)–Pb(2)–N(4)	89.6(3)	I(3)–Pb(2)–N(5)	70.4(3)
I(3)–Pb(2)–N(6)	84.1(3)	I(3)–Pb(2)–O(2)	148.2(2)
I(3)–Pb(2)–I(4)	101.08(3)	I(4)–Pb(2)–N(4)	150.7(3)
I(4)–Pb(2)–N(5)	141.4(3)	I(4)–Pb(2)–N(6)	71.5(3)
I(4)–Pb(2)–O(2)	96.8(3)	Ag(1)–I(1)–Ag(1)#1	109.63(6)
Ag(1)–I(1)–Ag(2)	70.18(4)	Ag(1)–I(1)–Ag(2)#1	70.33(4)

Ag(1)–I(1)–Ag(2)#2	179.75(12)	Ag(2)–I(1)–Ag(2)#1	109.86(6)
Ag(1)–I(2)–Ag(2)	74.88(4)	Ag(1)–I(2)–Pb(1)	102.51(5)
Ag(2)–I(2)–Pb(1)	81.72(5)	Ag(1)–I(3)–Ag(3)	115.08(7)
Ag(1)–I(3)–Pb(2)	108.02(5)	Ag(3)–I(3)–Pb(2)	88.07(3)
Ag(1)#2–I(4)–Ag(2)	75.13(4)	Ag(1)#2–I(4)–Pb(2)	83.13(5)
Ag(2)–I(4)–Pb(2)	102.93(5)	Ag(2)–I(5)–Ag(4)	116.13(7)
Ag(2)–I(5)–Pb(1)	75.35(4)	Ag(4)–I(5)–Pb(1)	81.18(2)

Symmetry transformations used to generate equivalent atoms: #1 –x+y+1, –x+1, z; #2 –y+1, x–y, z; #3 –y+1, x–y+1, z; #4 –x+y, –x+1, z; #5 –y, x–y, z; #6 –x+y, –x, z.

Table S7. Hydrogen Bond Lengths (Å) and Angles (deg) for **1**, **2**, **4**, **5** and **6**

D–H···A	d(H···A)	d(D···A)	<(DHA)
1			
N(1)–H(1A)···I(1)#1	3.23	3.936(10)	135.6
N(1)–H(1B)···I(3)#1	2.88	3.754(10)	162.4
N(3)–H(3A)···I(3)#2	3.01	3.848(9)	154.0
N(3)–H(3B)···I(3)#3	2.84	3.719(9)	162.0
N(4)–H(4A)···I(3)#1	3.19	3.908(9)	137.7
N(4)–H(4B)···I(2)#4	3.08	3.810(9)	138.2
2			
N(1)–H(1A)···I(3)#1	3.07	3.87(3)	149.6
N(1)–H(1B)···I(2)	3.29	3.86(3)	123.7
N(2)–H(2A)···I(2)#2	3.03	3.66(2)	128.9
N(2)–H(2A)···I(1)#3	3.08	3.75(2)	132.9
N(2)–H(2B)···I(3)#3	2.98	3.80(2)	152.5
4			
N(1)–H(1A)···I(2)#1	3.19	3.922(16)	138.8
N(1)–H(1B)···I(3)#3	3.04	3.797(15)	142.2
N(2)–H(2)···I(2)#2	2.93	3.752(13)	149.9
N(4)–H(4A)···I(1)	3.21	3.902(17)	134.5
N(4)–H(4B)···I(2)#1	2.94	3.820(17)	162.5
5			
N(1)–H(1A)···I(1)#1	3.30	4.113(17)	152.0
N(2)–H(2)···I(3)#2	2.97	3.822(16)	156.3
N(3)–H(3)···I(3)#3	3.03	3.832(17)	147.4
N(5)–H(5A)···I(4)	3.16	3.779(18)	127.8
N(5)–H(5A)···I(1)#1	3.20	3.789(15)	124.8
6			

N(1)–H(1A)···I(4)#1	2.87	3.739(14)	160.1
N(1)–H(1B)···I(2)#2	3.04	3.912(12)	160.8
N(2)–H(2)···I(5)#1	2.91	3.598(11)	132.7
N(3)–H(3A)···I(6)#3	3.14	3.917(15)	145.1
N(4)–H(4B)···I(8)	3.00	3.787(14)	146.5
N(5)–H(5)···I(3)	2.96	3.630(12)	130.7
N(6)–H(6A)···I(4)#4	2.97	3.831(12)	159.4
N(6)–H(6B)···I(2)	2.86	3.706(14)	155.5

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

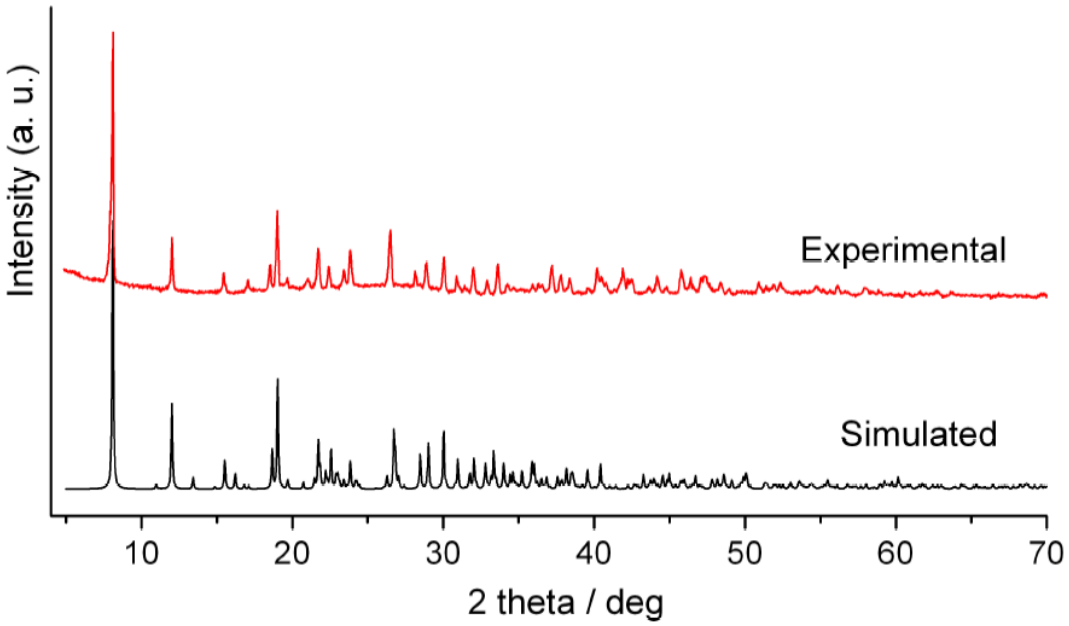

Figure S1. Powder X-Ray diffraction pattern (red) of the polycrystalline sample of compound **1** and the simulated pattern (black) base on the single crystal data.

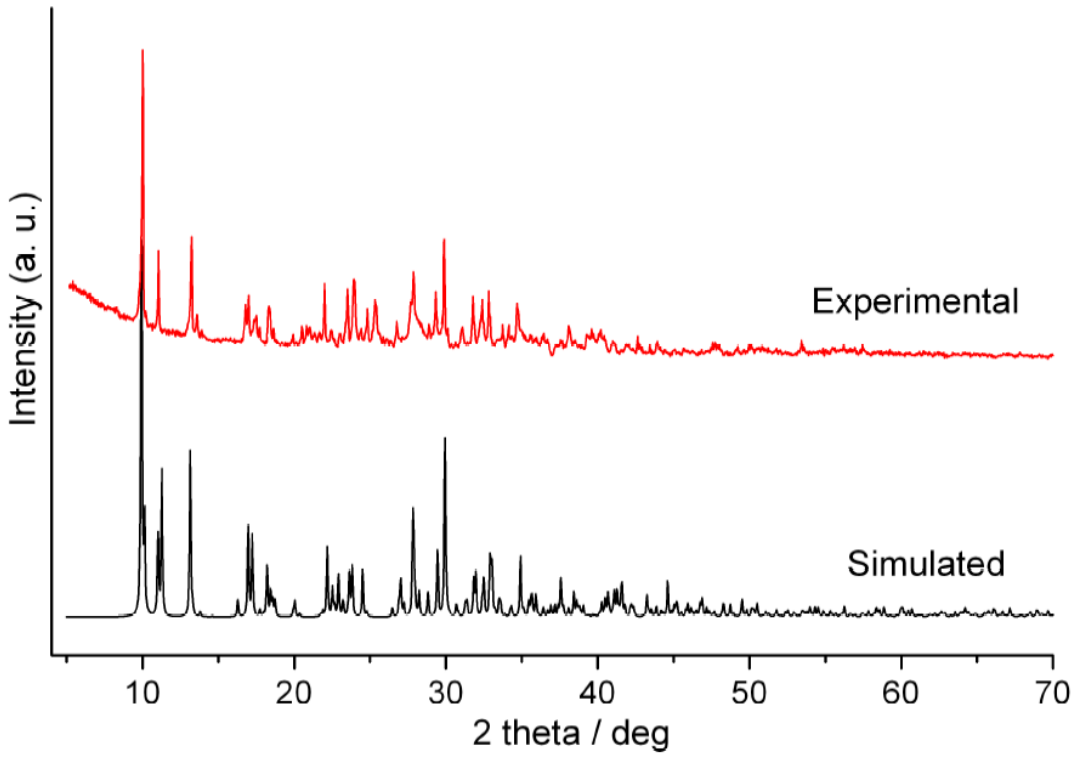

Figure S2. Powder X-Ray diffraction pattern (red) of the polycrystalline sample of compound **3** and the simulated pattern (black) base on the single crystal data.

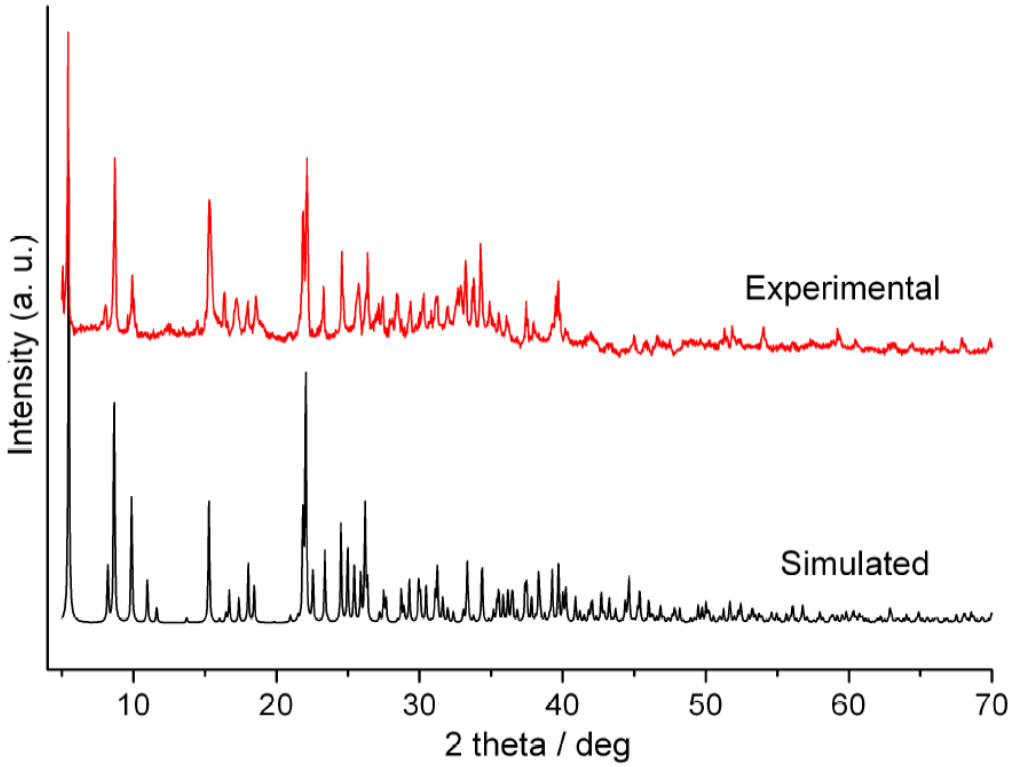

Figure S3. Powder X-Ray diffraction pattern (red) of the polycrystalline sample of compound **6** and the simulated pattern (black) base on the single crystal data.

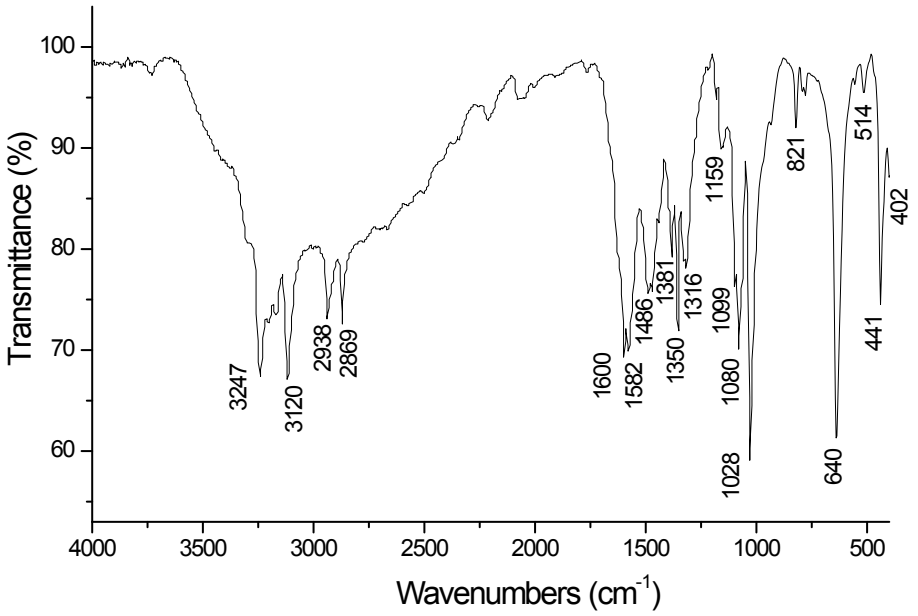

Figure S4. IR spectrum of complex **1**.

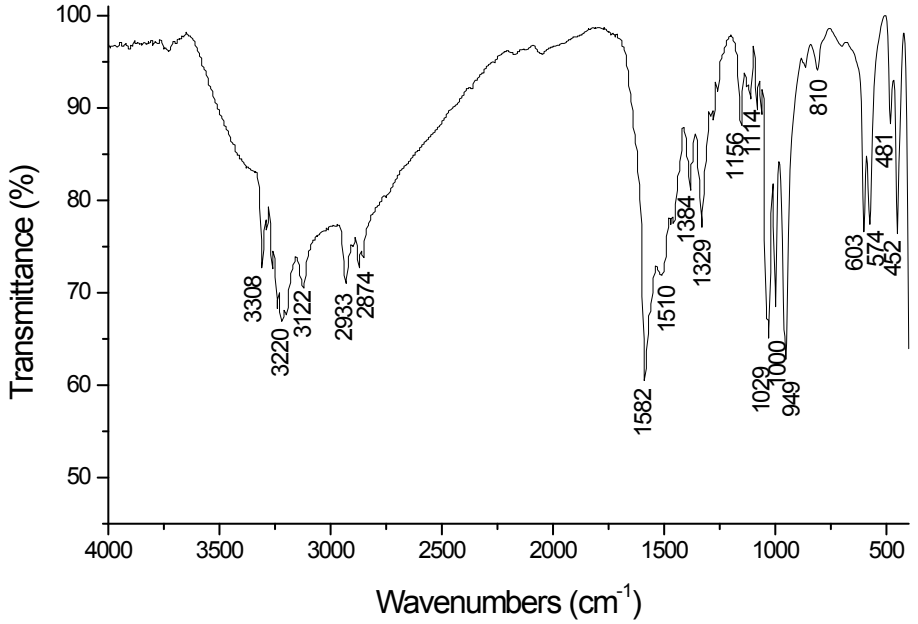

Figure S5. IR spectrum of complex **2**.

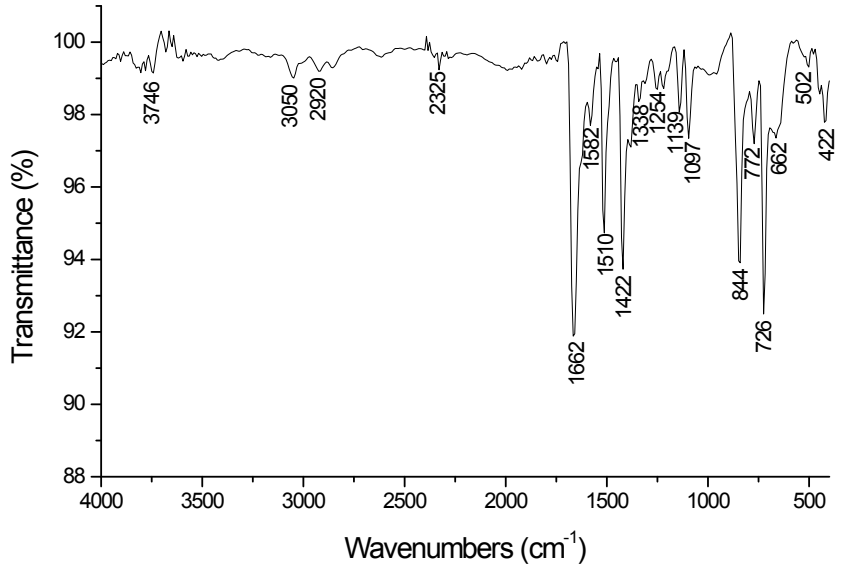

Figure S6. IR spectrum of complex **3**.

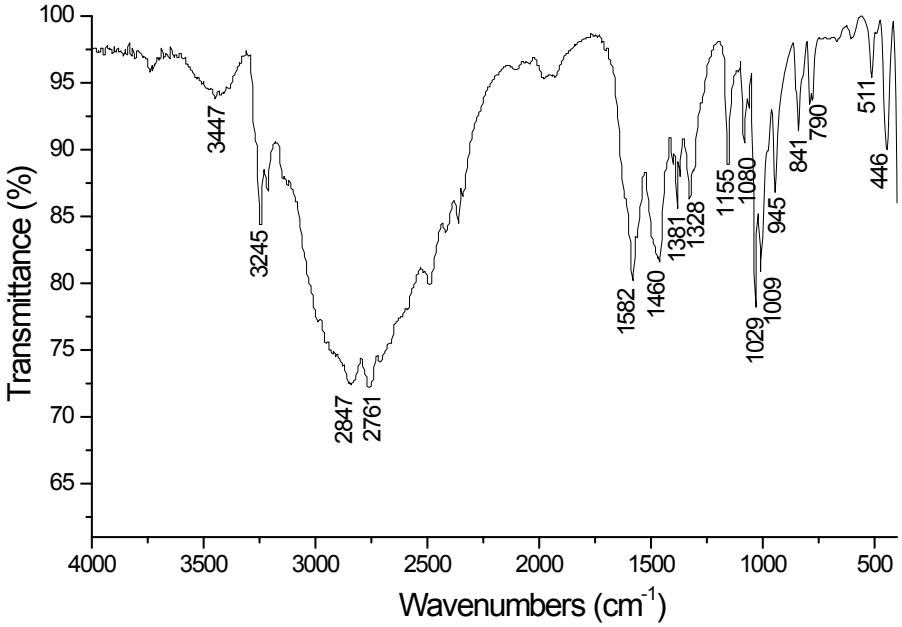

Figure S7. IR spectrum of complex **4**.

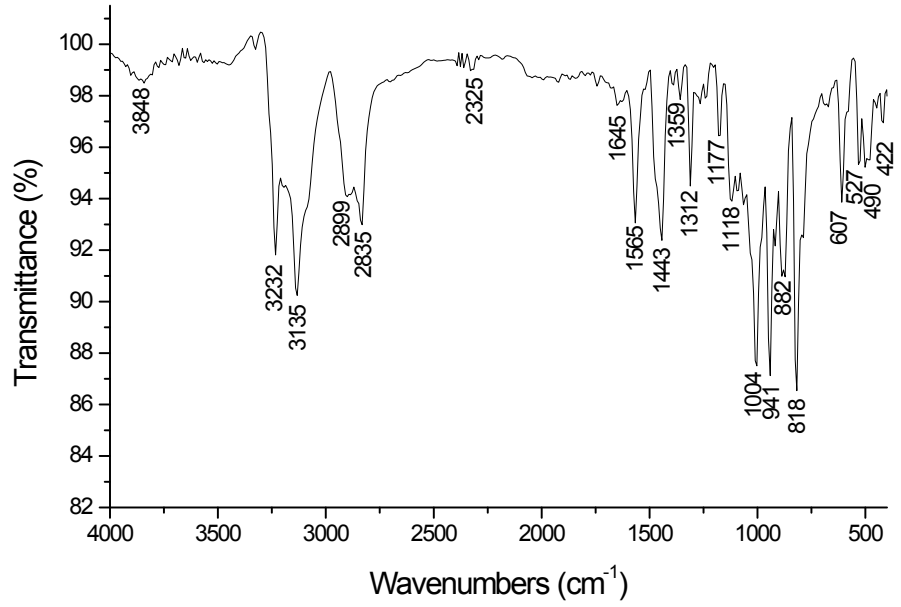

Figure S8. IR spectrum of complex **5**.

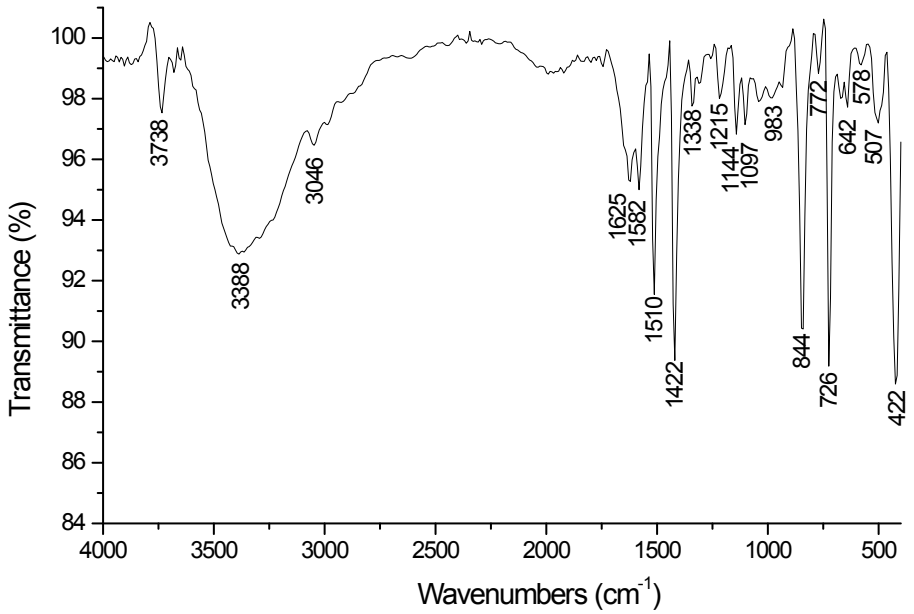

Figure S9 IR spectrum of complex **6**.

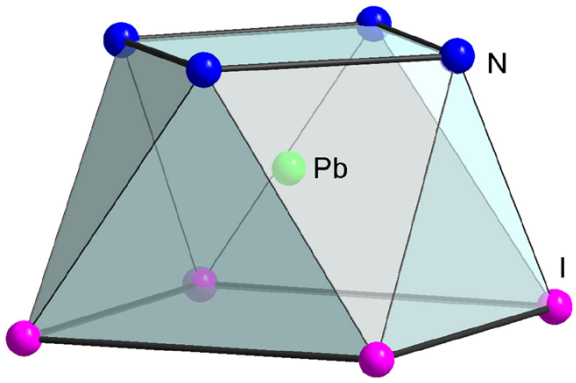

Figure S10. Coordination environment of the Pb^{2+} ion in **1**.

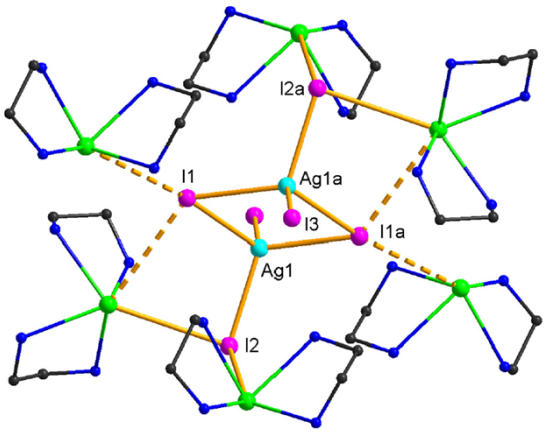

Figure S11. The connection between the Ag_2I_6 and $[Pb(en)_2]$ units in **1**.

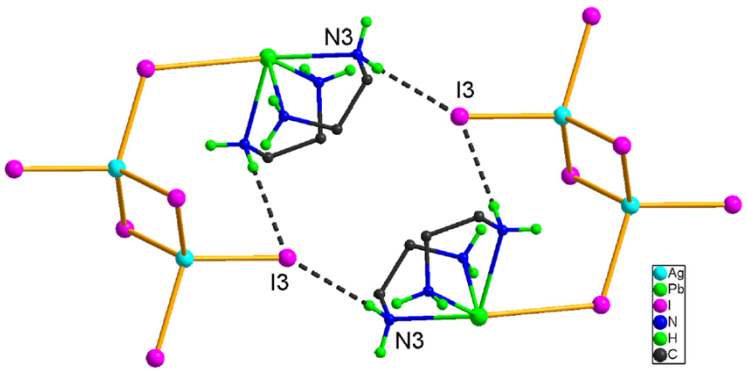

Figure S12. Intermolecular N–H···I hydrogen bonds in **1**.

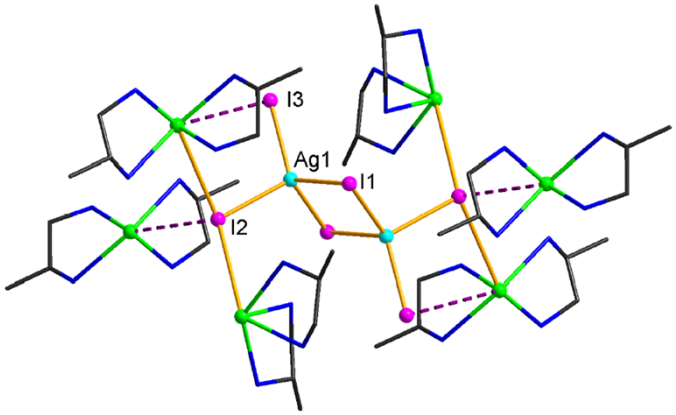

Figure S13. Connection between the Ag_2I_6 and $[Pb(pda)_2]^{2+}$ units in **2**.

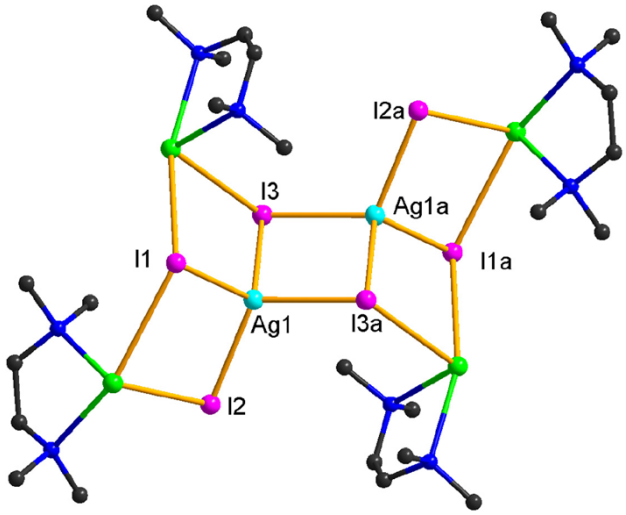

Figure S14. Connection between the Ag_2I_6 and $[Pb(tmeda)]^{2+}$ units in **3**.

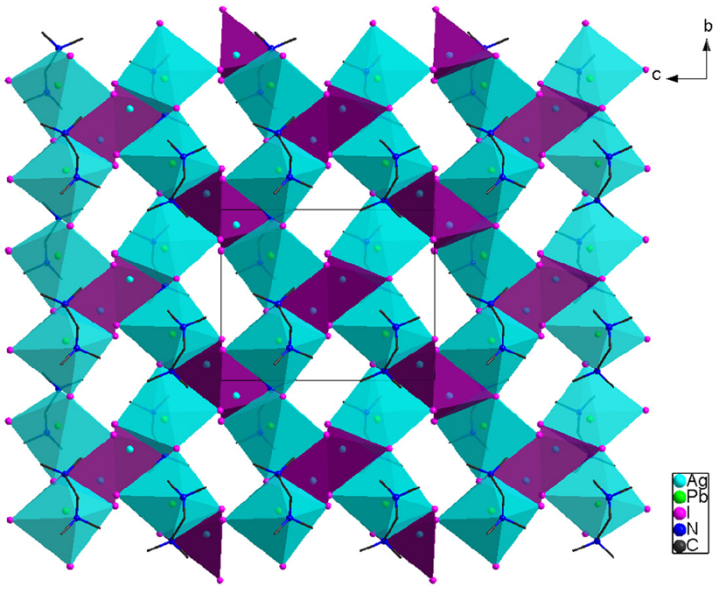

Figure S15. Polyhedral graph of **3** along the *b* axis. Hydrogen atoms are omitted for clarity.

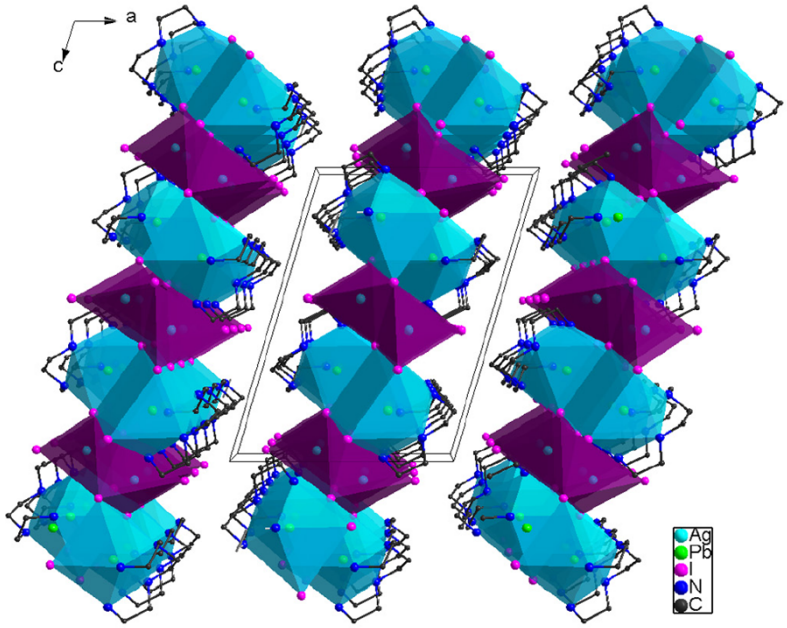

Figure S16. Polyhedral graph of **4** along the *b* axis. Hydrogen atoms are omitted for clarity.

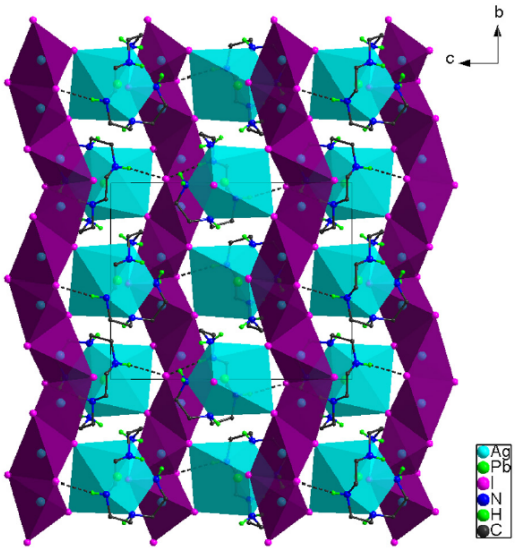

Figure S17. Polyhedral graph of **5** along the *a* axis. Hydrogen atoms are omitted for clarity.

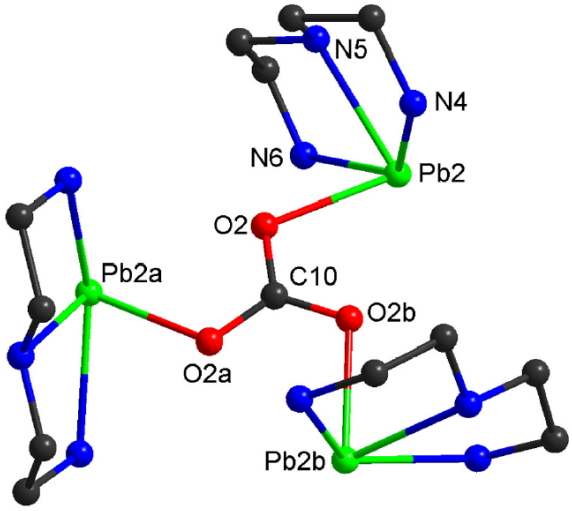

Figure S18. Crystal structure of the $[\{Pb(2)(dien)\}_3(\mu_3\text{-}CO_3)]^{4+}$ unit in **6** with labeling scheme.

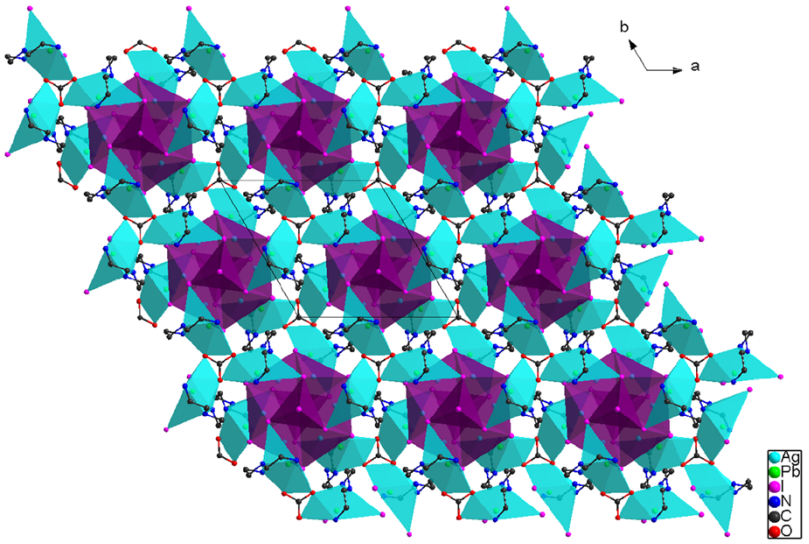

Fig. 19 Polyhedral graph of $[\{(dien)_3(CO_3)\}_2(Pb_6Ag_8I_{15})]_n^{n+}$ layer in **6** viewed along the *c* axis. $PbON_3I_2$ units are shown as blue octahedra, and AgI_4 are shown as purple tetrahedra

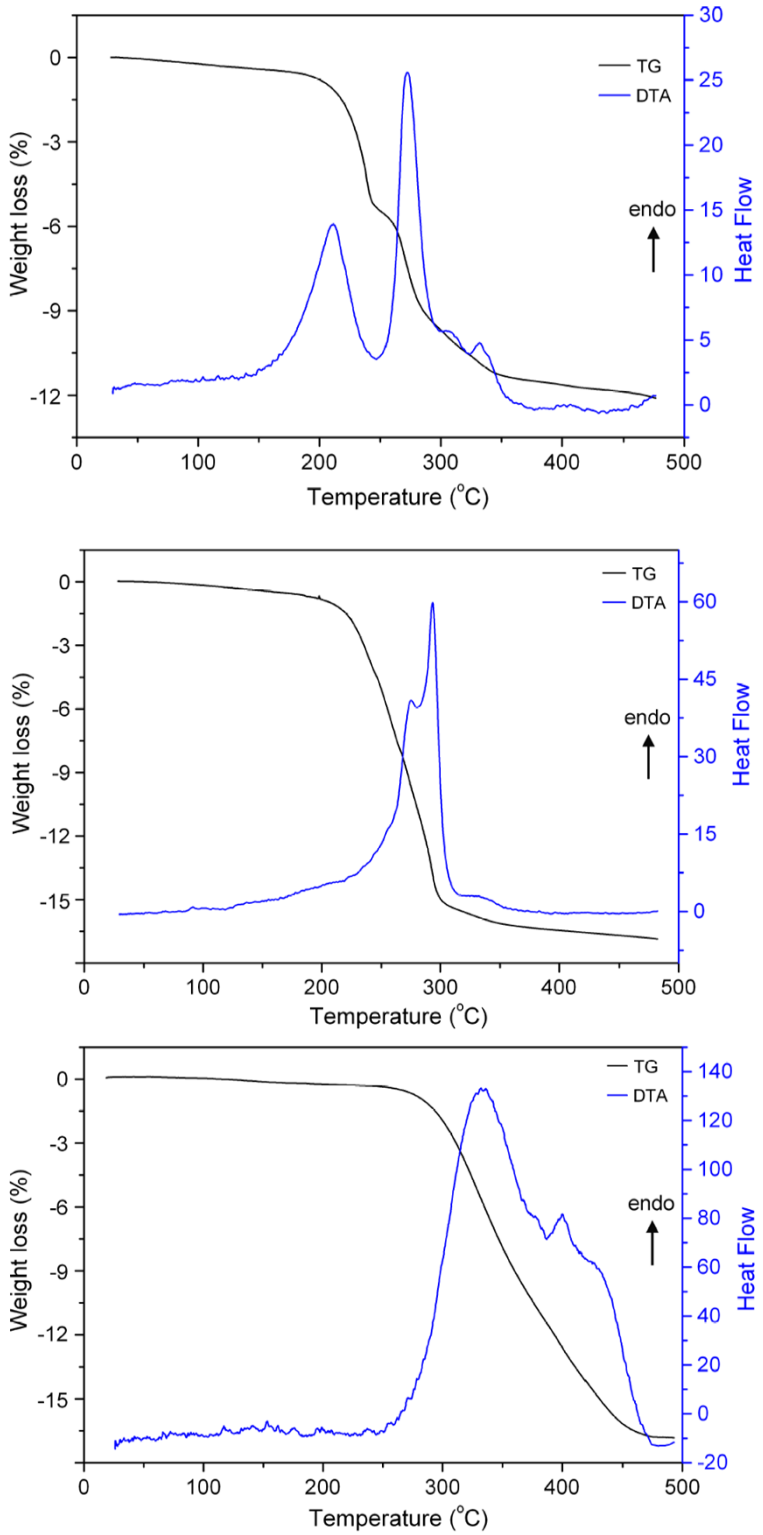

Figure S20. TG-DTA curves of compounds **1** (top), **4** (middle), and **5** (bottom).